Quantum Mechanics Part 1

Chapters 1-3

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Chapter 1 **Motivation, Motivation, Motivation .....**

In these notes we will develop a theory, which is deeply rooted in experiment and can only be understood using a new mathematical language. It not only describes how nature works in all microscopic physical systems, but also in macroscopic physical systems.

It is most important, however, when the characteristic length scale of the physical system is smaller than $10^{-4}\,m$.

This theory is called **quantum mechanics**.

The physical world we will discover in our studies is a strange and fascinating place where nature operates in a way that seems to defy the intuition we have built up living among macroscopic systems. We will not endeavor to explain why nature works in this particular way since it is my strong belief, as we will see in this book, that it is not possible to do so within the context of this theory.

We will, however, be able to correctly predict the outcomes of an amazingly wide range of experiments in many different fields of physics, chemistry and biology.

Let me emphasize my strong belief that theories in physics should only endeavor to make predictions about experimental measurements and not attempt to provide reasons for *why* nature works in these particular ways, that is, why we must choose to start with certain postulates.

Feynman put it best.....

We know how the electrons and light behave. But what can I call it? If I say they behave like particles I give the wrong impression; also if I say they behave like waves. They behave in their own inimitable way, which technically could be called a quantum mechanical way.

They behave in a way that is like nothing that you have seen before. Your experience with things that you have seen before is incomplete. The behavior of things on a very small scale is simply different. An atom does not behave like a miniature representation of the solar system with little planets going around in orbits. Nor does it appear like a cloud or fog of some sort surrounding the nucleus. It behaves like nothing you have ever seen before.

There is one simplification at least. Electrons behave in this respect exactly the same way as photons; they are both screwy, but in exactly the same way.

The difficulty really is psychological and exists in the perpetual torment that results from your saying to yourself "but how can it really be like that?", which is a reflection of an uncontrolled but vain desire to see it in terms of something familiar.

I will not describe it in terms of an analogy with something familiar; I will simply describe it...

I am going to tell you what nature behaves like. If you will simply admit that maybe she does behave like this, you will find her a delightful and entrancing thing. Do not keep saying to yourself, if you can avoid it, "but how can it really be like that?" because you will get "down the drain", into a blind alley from which nobody has yet escaped.

Nobody knows how it can be like that.

and we can add an addendum .....

and "nobody knows why it is like that"

We will not be able to reduce the quantum universe to everyday ways of thinking(usually called *common sense*).

In fact, in order to understand the ideas and implications of the theory we will have to adjust all of our ways of thinking at the most fundamental level.

Imagine, for a moment, that you are attempting to understand a new culture. If you are serious about it, the first thing you would do is to learn the language appropriate to that culture so that you can put your experiences in the proper context. Understanding the universe of quantum phenomena is much like a understanding a new culture where the appropriate language is mathematics and the experiences we are attempting to put into context are experiments.

As we shall see, we will have to use a mathematical language to describe the quantum world since ordinary language, which was developed to explain everyday occurrences(experiments on macroscopic objects), will turn out to be totally inadequate.

Since it makes no sense to attempt any understanding of the nature of quantum phenomena without first learning to speak and use the language of the quantum world, we will spend the first several chapters of this book learning the appropriate mathematics, in particular, the subject of linear vector spaces.

The adjustment of our ways of thinking at the fundamental level that will be needed is not simply a mathematical matter, however. The development of the necessary mathematical language will not come into conflict with our everyday modes of thinking in any major way. Although, the mathematics of linear vector spaces is very elegant, you will be able to understand it without much difficulty and without having your basic view of the world changed at any fundamental level.

You will be troubled, however, when we apply the mathematics to physical systems that develop according to quantum ideas. We will attach physical meaning to the mathematical formalism in ways that will conflict with your well-developed views(I will call these classical views) about how the world works.

We will rethink both mathematics and quantum theory using the Dirac language, which, as we shall see, incorporates the very nature of the quantum world in an intrinsic and natural way. Since we are attempting to develop a physical theory, we will link all the mathematical concepts that we introduce to physical concepts as we proceed.

Dirac was able to link the physical structure of quantum mechanics with the mathematical structure in a unique way. His mathematical language incorporates the physical meaning directly into the formalism and the calculational methods. The language explicitly exhibits the physics and clearly exposes the internal logic of quantum mechanics. Once we understand the language, every equation will directly convey its physical meaning without the need for further explanation or any need for inadequate models.

It is very important to understand that the Dirac language is not simply a new notation for quantum mechanics(as many physicists seem to think).

It is a way of thinking about quantum mechanics. It will allow us to use the physical ideas of quantum mechanics to develop the appropriate mathematical language rather than the other way around. This will allow the very mathematical quantum theory to be more closely connected to experiment than any other physical theory.

These statements about the importance of understanding the mathematical language appropriate to the physics under consideration do not only apply to the quantum world. It is true for all areas of physics and other sciences. One should always learn the appropriate language before studying any field that relies on that language for its understanding.

Mathematical Methods

As I stated, will have to use various mathematical techniques in order to formulate quantum mechanics and in order to solve the resulting equations.

Some of these techniques you have may have learned in a Mathematical Methods in Physics course, some you may have learned in Mathematics courses such as Linear Algebra, and Multivariable Calculus and some we will develop in this book.

The techniques we will need are linear operators in Hilbert space (an extension of linear algebra), partial differential equations, special functions of mathematical physics (Legendre polynomials, spherical harmonics, Bessel functions), Fourier transforms, use of Green's functions, integral equations, contour integration in the complex plane, group theory and group representations, etc. We will cover many of these techniques in detail as we proceed.

As we proceed we will cover many applications of quantum theory to physical systems in the areas of atomic and molecular physics.

Chapter 2 **The Mathematics of Quantum Physics: Dirac Language**

Because it is so important, I repeat that this study of the mathematics of quantum mechanics assumes that you have a good background in the following areas:

- Calculus
  Differentiation and integration
- Infinite series
  Taylor and power series
- Linear Algebra
  Linear vector spaces and matrices
- Multivariable Calculus
  Partial derivatives
  Gradient, divergence, curl and Laplacian
- Mathematical Methods
  Ordinary and partial differential equations
  Fourier series and Fourier transforms

This study of the mathematical formalism of quantum theory will center around the subject of linear vector spaces. We will present this subject using Dirac language and connect it to the physics as we proceed. At the start of our discussion, we will mix standard mathematical notation and the Dirac language so that the transition to using only the Dirac language will be easier.

Quantum systems cannot be described in terms of our everyday experience. To understand them it is necessary to use the abstract language provided by the algebra of linear operators on Hilbert space.

When we present the mathematical formalism appropriate to a physical theory we have two choices.

We can approach the subject abstractly and deal directly with mathematical quantities of fundamental importance or we can choose a particular a particular representation (abstract coordinate system) and work with the numbers (functions) that correspond to the fundamental quantities in that coordinate representation.

We will follow the abstract approach in most cases since it will allow us to delve more deeply into the fundamental nature of the physical theory and, in addition, enable us to treat the physical laws in a precise and efficient manner.

First let us define *mappings* which are used almost everywhere in the discussion, sometimes explicitly and sometimes implicitly.

2.1 **Mappings**

Given two sets A and B, let $a \in A$, $b \in B$. A mapping T from A to B:

$$a \mapsto b = Ta \tag{2.1}$$

can be of the following types:

1. T is a mapping of A *into* B if to each $a \in A$ there corresponds a definite element $Ta \in B$(there may be elements of B that do not correspond to any element of A and different elements of A may correspond to the same element of B). The range of the mapping is the subset $TA \subset B$ (TA is a subset set of B but not equal to B) formed by those elements that correspond to some elements of A.

2. T is a mapping of A *onto* B if to each element of A there corresponds a definite element $Ta \in B$ and to every element of B there corresponds at least one element of A (in this case $Ta = B$).

3. A *one-to-one* mapping is where distinct elements of A correspond to distinct elements of B: $Ta \neq Tb$ if $a \neq b$.

4. It follows that if T is a one-to-one mapping from A *onto* B, then there exists an inverse one-to-one mapping T^{-1} from B *onto* A. Such an inverse does not exist if T is a one-to-one mapping A *into* B.

2.2 **Linear Vector Spaces**

The mathematical formalism of quantum mechanics is based on the theory of linear vector spaces. In this chapter we shall present a complete exposition of the mathematics of linear vector spaces. We shall state theorems without proofs (excellent proofs are available in a variety of texts). Instead of proofs, we shall relate the theorems where appropriate to the physics of quantum mechanics using the Dirac language and provide concrete examples that will help us understand the physical content in our later discussions.

The number of configurations experimental instruments can exhibit is finite.

This implies that, in principle, only the language of finite-dimensional vector spaces will be needed to explain experimental results and to understand the theoretical structure of quantum mechanics. However, if we want to embed the theory in a spacetime continuum, then it will be necessary to consider idealized instruments capable of an infinite number of configurations. This will require a description using the language of infinite-dimensional spaces, in particular the use of a vector space called a non-separable or rigged Hilbert space. Because these idealized infinite instruments are approximations of the actual finite ones, physicists usually ignore those properties of the infinite-dimensional Hilbert space that cannot be derived from the properties of finite-dimensional spaces by some, not necessarily unique, physically based limiting procedure.

A working knowledge of the mathematical description that results from the adopted limiting procedure is necessary to understand many of the developments of quantum mechanics.

The following mathematical presentation reflects these considerations. The results pertaining to finite-dimensional spaces, necessary for the understanding of the structure of quantum mechanics, are presented with thoroughness. The generalization to infinite-dimensional spaces, which is a very difficult task, is discussed in less detail.

These mathematical details are usually ignored in most textbooks, which I believe makes it very difficult to understand the fundamental ideas underlying quantum mechanics.

In most of our discussions we can assume we are in a finite-dimensional vector space and the results will generalize without change to the Hilbert space case. We will deal with the special problems associated with the infinite dimensionality of Hilbert space as they arise.

2.3 **Linear Spaces and Linear Functionals**

A vector space is defined with reference to a field. We consider the case where the field is the field C of complex numbers because this is the case of interest in quantum mechanics.

Ket Vectors

The mathematical vectors that will allow us to describe physical states will be called *ket vectors* or *kets* and be represented by the symbol $|\ldots\rangle$ (due to Dirac). We will label different vectors(states) according to their associated physical(measurable) properties and these will be inserted inside the ket symbol $|a, b, ...\rangle$. The ket vectors will form the basis for the Dirac language of the associated vector space defined below. These simple mathematical objects will turn out to have sufficient mathematical structure to allow us to represent all of the important features of quantum theory in terms of them.

Whether these mathematical objects have any objective physical content themselves must be discussed later as we develop the theory.

At this point, however, let us state a couple of the basic properties of the ket vectors and their connection to physics to help set the stage for the discussion that will follow.

As with any other vectors, kets can be multiplied by complex numbers and can be added together to get another ket vector

$$c_1 |a\rangle + c_2 |b\rangle = |q\rangle \tag{2.2}$$

where c_1 and c_2 are complex numbers.

The crucial assumptions we will make later as we connect the Dirac language, the mathematical formalism and the physics are:

- Each state of a physical system at a given time can be mathematically described by a definite ket vector. There is some correspondence!
- If a physical state is a superposition(sum) of other physical states, its corresponding ket vector is a linear sum(combination) of the ket vectors corresponding to the other states

The state $|q\rangle$ in (2.2) is a superposition of the states $|a\rangle$ and $|b\rangle$ with the mathematical properties of this superposition defined precisely by the two complex numbers c_1 and c_2. For example, the state of a photon passing through a double-slit apparatus might be described by the superposition

$$|photon\ in\ 2-slit\ apparatus\rangle = a\,|slit\ 1\rangle + b\,|slit\ 2\rangle \qquad (2.3)$$

where $|slit\ 1\rangle$ is the state of a photon that passes through slit 1.

With these tantalizing thoughts rambling about in your minds, let us turn to the mathematical formalism.

Definition:

A *linear vector space* V is a set of abstract elements, called *vectors*,

$$|1\rangle, |2\rangle, \ldots, |M\rangle, \ldots, |N\rangle, \ldots \tag{2.4}$$

for which there exists two rules:

1. a rule for creating a vector sum or vector addition,

$$|7\rangle + |12\rangle$$

2. a rule for multiplication of a vector by a complex scalar c,

$$c\,|13\rangle$$

The following properties hold:

1. the result of applying either or both of these rules is another vector in the same space; this is called *closure*

$$c_1 |7\rangle + c_2 |12\rangle \in V$$

2. scalar multiplication is *distributive* with respect to the vectors

$$c(|7\rangle + |12\rangle) = c|7\rangle + c|12\rangle$$

3. scalar multiplication is *associative*

$$c_1(c_2|7\rangle) = c_1 c_2 |7\rangle$$

4. addition is *commutative*

$$|7\rangle + |12\rangle = |12\rangle + |7\rangle$$

5. addition is *associative*

$$|6\rangle + (|7\rangle + |12\rangle) = (|6\rangle + |7\rangle) + |12\rangle$$

6. there exists a unique *zero* or *null* vector $|\varnothing\rangle$ such that

$$|7\rangle + |\varnothing\rangle = |7\rangle \text{ and } 0|M\rangle = |\varnothing\rangle$$

7. for every vector $|M\rangle$ there exists a unique additive *inverse* vector $|-M\rangle$ where

$$|M\rangle + |-M\rangle = |\varnothing\rangle \text{ and } |-M\rangle = -|M\rangle$$

Example: Consider the set of all *3-tuples*, which is a particular example of a finite-dimensional vector space

$$|i\rangle = \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix} \tag{2.5}$$

Addition is defined by

$$|i\rangle + |i\rangle = \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix} + \begin{pmatrix} a_j \\ b_j \\ c_j \end{pmatrix} = \begin{pmatrix} a_i + a_j \\ b_i + b_j \\ c_i + c_j \end{pmatrix} \tag{2.6}$$

Multiplication by a scalar q is defined by

$$q\,|i\rangle = \begin{pmatrix} qa_i \\ qb_i \\ qc_i \end{pmatrix} \tag{2.7}$$

The null vector is defined by

$$|\varnothing\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.8}$$

We must emphasize that use of the word "vector" here is not meant to imply that we are talking about a mathematical object that in any way needs to possess properties such as magnitude and direction. These "vectors" are abstract mathematical objects whose properties are defined above.

Other examples are: 1. the set of all functions $f(x)$ of a real variable x for which

$$\int \mid f(x) \mid^2 \, dx < \infty$$

with addition and multiplication by a scalar defined by

$$(f+g)(x) = f(x) + g(x) \, and \, (af)(x) = af(x)$$

This space is called L^2.

2. the set of all infinite sequences of numbers
$x = (x_1, x_2, x_3, \ldots, x_i, \ldots)$ such that

$$x + y = (x_1 + y_1, x_2 + y_2, x_3 + y_3, \ldots, x_k + y_k, \ldots)$$

with addition and multiplication by a scalar defined by

$$(f + g)(x) = f(x) + g(x) \qquad (af)(x) = af(x)$$

$$ax = (ax_1, ax_2, ax_3, \ldots, ax_k, \ldots)$$

3. the set of all $2x2$ matrices

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

with addition and multiplication by a scalar defined by

$$A + B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11} + b_{11} & a_{12} + b_{12} \\ a_{21} + b_{21} & a_{22} + b_{22} \end{pmatrix}$$

$$cA = c \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} ca_{11} & ca_{12} \\ ca_{21} & ca_{22} \end{pmatrix}$$

These examples should make it clear that it is important, as we have emphasized already, not to think about magnitudes and directions as being the defining properties of "vectors" in any way. We must be very careful not to attribute any specific properties derived from special examples as general properties of vectors in any abstract vector space.

Isomorphism -Two vector spaces U and V (defined over the same field) are said to be *isomorphic* if there exists a one-to-one and onto correspondencex$u \leftrightarrow v$ between every vector $u \in U$ and every other vector $v \in V$ that preserves the linear operations, that is, $\alpha u_1 + \beta u_2 \leftrightarrow \alpha v_1 + \beta v_2$ whenever $u_1 \leftrightarrow v_1$ and $u_2 \leftrightarrow v_2$ for $u_1, u_2 \in U$ and $v_1, v_2 \in V$. Such a correspondence is called an *isomorphism*. If one is only interested in linear operations on vectors, then two isomorphic spaces are indistinguishable from each other.

Definition: A set of vectors is said to be *linearly independent* if a linear relation of the form

$$\sum_{k=1}^{n} c_k \left|k\right\rangle = \left|\varnothing\right\rangle \tag{2.9}$$

implies that $c_k = 0$ for all k; otherwise the set of vectors is *linearly dependent*.

If a set of vectors is linearly dependent, then we can express a member of the set as a linear combination of the other members of the set.

Examples:

1. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

This set is linearly independent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = |\varnothing\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

implies that the only solution is

$$a_1 = a_2 = a_3 = 0$$

2. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

This set is linearly independent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ a_1 \\ 0 \end{pmatrix} + \begin{pmatrix} a_2 \\ -a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix}$$

$$= \begin{pmatrix} a_1 + a_2 \\ a_1 - a_2 \\ a_3 \end{pmatrix} = |\varnothing\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

implies that the only solution is

$$a_1 + a_2 = a_1 - a_2 = a_3 = 0 \qquad \text{or} \qquad a_1 = a_2 = a_3 = 0$$

3. Consider the set of vectors(3-tuples in this case)

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}$$

This set is linearly independent since

$$a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ a_1 \\ a_1 \end{pmatrix} + \begin{pmatrix} a_2 \\ -a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 2a_3 \\ 0 \\ a_3 \end{pmatrix}$$

$$= \begin{pmatrix} a_1 + a_2 + 2a_3 \\ a_1 - a_2 \\ a_1 + a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

implies that the solution is

$$a_1 + a_2 + 2a_3 = a_1 - a_2 = a_1 + a_3 = 0 \qquad \text{or} \qquad a_2 = a_1, a_3 = -a_1$$

Note: For simplicity and in all cases where no ambiguity will arise, we will simplify the notation for the "null" vector from now on. We will write

$$\sum_{k=1}^{n} c_k \left|k\right\rangle = 0 \qquad \text{instead of} \qquad \sum_{k=1}^{n} c_k \left|k\right\rangle = \left|\varnothing\right\rangle \tag{2.10}$$

We say that an infinite set of vectors is linearly independent if **every finite subset** is linearly independent. Alternatively, we can use this method: if the determinant of the matrix formed by using the vectors as columns is equal to zero, then the vectors are linearly dependent.

Definition: The maximum number of linearly independent vectors in a space V is called the *dimension* of the space $dim(V)$.

Definition: A set of vectors $|k\rangle, k = 1, 2, 3, \ldots, n$ *spans* the space if every vector $|Q\rangle$ in the space can be written as a linear combination of vectors in the set

$$|Q\rangle = \sum_{k=1}^{n} q_k |k\rangle \tag{2.11}$$

This linear combination, which is given by the coefficients $q_k, k = 1, 2, \ldots, n$ is unique.

Definition: A set of vectors is a *basis* for the space if it is a linearly independent set *and* spans the space, that is, if $dim(V) = m$, a set of m linearly independent vectors is called a *basis* on V.

The set of vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2.12}$$

is the *maximal* set of linearly independent vectors since any other vector $|g\rangle$ in the space can always be written as a linear combination of them as

$$|g\rangle = a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \tag{2.13}$$

Therefore the dimension of this vector space is 3. This set of vectors is also a basis. The basis is *not unique* since the set of linearly independent vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2.14}$$

also spans the space, i.e.,

$$|g\rangle = c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} c_1 + c_2 \\ c_1 + c_2 \\ c_3 \end{pmatrix} \tag{2.15}$$

implies that

$$2c_1 = a_1 + a_2 \quad 2c_2 = a_1 - a_2 \quad c_3 = a_3 \tag{2.16}$$

and, thus, this set is also a basis. Clearly, a basis spans the whole of V.

Definition: The coefficients q_k in the expansion of an arbitrary vector $|Q\rangle$ in terms of a basis set $|k\rangle, k = 1, 2, 3, \ldots, n$

$$|Q\rangle = \sum_{k=1}^{n} q_k |k\rangle \tag{2.17}$$

are called the *components* of the vector $|Q\rangle$ in that basis.

Example: In the space of 3-tuples, a basis is represented by the three vectors

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2.18}$$

so that an arbitrary vector in the space can be written

$$|g\rangle = a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle = \begin{pmatrix} a_1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ a_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \tag{2.19}$$

so that a_1, a_2 and a_3 are the components.

When we add vectors(must be defined with respect to the same basis) we simply add their components

$$|Q\rangle + |R\rangle = \sum_{k=1}^{n} q_k |k\rangle + \sum_{k=1}^{n} r_k |k\rangle = \sum_{k=1}^{n} (q_k + r_k) |k\rangle \qquad (2.20)$$

Subspaces - A subset of a vector space V, which is also a vector space, is a *subspace*, that is, it contains all the linear combinations of any number of its vectors - it said to be *closed*. The smallest subspace that contains the set S of vectors is said to be *spanned* by S. We note that the intersection $M \cap N$ - in the sense of set theory - of two subspaces M and N is a subspace, but, in general, their union $M \cup N$ is not.

2.4 **Inner Products**

The vector spaces we have been discussing do not need to contain vectors that have a well-defined length or direction in the ordinary sense (remember the example of the $2x2$ matrices). We can, however, define *generalizations* of length and direction in an arbitrary space using a mathematical object called the *inner product*. The inner product is a generalization of the standard dot product. I will first discuss the inner product using *standard* mathematical notation and then return to the *Dirac language*.

Definition: An *inner product* for a linear vector space associates a scalar (f, g) with every *ordered pair* of vectors f, g. It satisfies these properties: 1.

$$(f, g) = \text{ complex number}$$

2.

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

3.

$$(f, c_1 g_1 + c_2 g_2) = c_1 (f, g_1) + c_2 (f, g_2)$$

4.

$$(f, f) \geq 0 \text{ with equality if and only if } f = \text{ null vector}$$

Now (2) and (3) above imply that

$$(c_1 g_1 + c_2 g_2, f) = c_1^* (f, g_1) + c_2^* (f, g_2) \tag{2.21}$$

Hence, the inner product is said to be *linear* in its *second* argument and *antilinear* in its *first* argument.

Definition: The non-negative number $\|f\| = (f, f)^{1/2}$ is called the *norm* or *length* of the vector f. Clearly, $\|f\| = 0$ if and only if $f = 0$.

Definition: If the inner product of two vectors is zero, then the vectors are *orthogonal*.

Definition: A set of vectors $\{f_i\}$ is said to be *orthonormal* if the vectors are pairwise orthogonal and of unit norm. We can summarize this property by the equation

$$(f_i, f_j) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \tag{2.22}$$

where the symbol δ_{ij} is called the *Kronecker delta*.

Schwarz's Inequality: scalar products satisfy

$$| (f, g) |^2 \leq (f, f)(g, g) \tag{2.23}$$

Triangle Inequality: scalar products satisfy

$$\|(f + g)\| \leq \|f\| + \|g\| \tag{2.24}$$

Equality holds in both cases only if one vector is a scalar multiple of the other, i.e., $f = cg$ where the scalar c is real and positive.

An inner product space is simply one in which an inner product is defined. A *unitary* space is a finite-dimensional inner product vector space. In fact, every finite-dimensional space can be made into a unitary space.

Examples:

1. For the case of n-tuples(an n-dimensional vector space)

$$f = (x_1, x_2, x_3, \ldots, x_n), \quad , \quad g = (y_1, y_2, y_3, \ldots, y_n)$$

$$(f, g) = \sum_{k=1}^{n} x_k^* y_k$$

2. For the case of square integrable functions

$$(f, g) = \int f^*(x) g(x) w(x)\, dx$$

where $w(x)$ is a nonnegative weight function.

When a vector Q is expanded as a linear combination

$$Q = \sum_k q_k f_k \tag{2.25}$$

of orthonormal basis vectors f_k, the coefficients or components are given by the inner product, i.e.,

$$(f_j, Q) = \sum_k q_k (f_j, f_k) = \sum_k \delta_{kj} = q_j \tag{2.26}$$

or

$$Q = \sum_k (f_k, Q) f_k \tag{2.27}$$

Of the two basis vector sets for the 3-dimensional vectors we looked at earlier:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2.28}$$

is an orthonormal basis and

$$|1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{2.29}$$

is orthogonal but not orthonormal.

For later use we note the following.

Given two unitary spaces U and V, their *direct sum* $W = U \oplus V$ is the unitary space consisting of the pairs $\{f.g\}$ written $f \oplus g, f \in U, g \in V$ with the operations defined by

$$\alpha_1 f_1 \oplus g_1 + \alpha_2 f_2 \oplus g2 = (\alpha_1 f_1 + \alpha_2 f_2) \oplus (\alpha_1 g_1 + \alpha_2 g_2) \tag{2.30}$$

$$(f_1 \oplus g_1, f_2 \oplus g2) = (f_1, f_2) + (g_1, g_2) \tag{2.31}$$

This is a definition that can clearly be extended to any finite number of spaces.

2.5 **Linear Functionals**

Linear complex-valued functions of vectors are called *linear functionals* on V. A linear functional Γ assigns a scalar value $\Gamma(f)$ to each vector f in the vector space V, such that linearity holds

$$\Gamma(c_1 f_1 + c_2 f_2) = c_1 \Gamma(f_1) + c_2 \Gamma(f_2) \tag{2.32}$$

for any vectors f_1 and f_2 and any scalars c_1 and c_2.

The set of linear functionals on V form a linear space V' where we define addition and scalar multiplication by

$$(\Gamma_1 + \Gamma_2)(f) = \Gamma_1(f) + \Gamma_2(f) \tag{2.33}$$

$$(c\Gamma)(f) = c\Gamma(f) \tag{2.34}$$

The vector space V' is called the *dual space* of the vector space V.

There is a one-to-one correspondence between linear functionals Γ in V' and the vectors f in V, such that the linear functional associated with f has the form

$$\Gamma_f(g) = (f, g) \tag{2.35}$$

where f is a fixed vector and g is an arbitrary vector. This is called the *Riesz theorem*.

Using the properties of the inner product we can show that

$$\Gamma_f + \Gamma_g = \Gamma_{f+g} \qquad \text{and} \qquad a\Gamma_f = \Gamma_{a^* f} \tag{2.36}$$

or

$$\Gamma_f(h) + \Gamma_g(h) = \Gamma_{(f+g)}(h) \tag{2.37}$$

$$(f,h)+(g,h)=(f+g,h) \tag{2.38}$$

and

$$a\Gamma_f(h)=a(f,h)=(a^*f,h)=\Gamma_{a^*f} \tag{2.39}$$

The scalar product is clearly *antilinear* in Γ and linear in f.

The vector f that corresponds to a given linear functional Γ_f is easily found by direct construction.

Let $\{\alpha^i\}$ be a set of orthonormal basis vectors in V (this means that $(\alpha_i,\alpha_j)=\delta_{ij}$, and let

$$\phi=\sum_n c_n\alpha_n \tag{2.40}$$

be an arbitrary vector in V. Then we have from its definition

$$\Gamma_f(\phi)=\Gamma_f\left(\sum_n c_n\alpha_n\right)=\sum_n c_n\Gamma_f(\alpha_n) \tag{2.41}$$

We now choose

$$f = \sum_n [\Gamma_f(\alpha_n)]^* \alpha_n \tag{2.42}$$

Its inner product with the arbitrary vector ϕ is

$$(f, \phi) = \left(\sum_n [\Gamma_f(\alpha_n)]^* \alpha_n, \sum_m c_m \alpha_m \right) = \sum_{n,m} [\Gamma_f(\alpha_n)] c_m (\alpha_n, \alpha_m) \tag{2.43}$$

$$= \sum_{n,m} [\Gamma_f(\alpha_n)] c_m \delta_{nm} = \sum_n [\Gamma_f(\alpha_n)] c_n = \Gamma_f(\phi) \tag{2.44}$$

So the vector f corresponding to Γ_f is given by

$$f = \sum_n [\Gamma_f(\alpha_n)]^* \alpha_n \tag{2.45}$$

2.6 **The Dirac language of Kets and Bras**

Let us rewrite everything we have done so far in the Dirac language.

Vectors in the linear space V are called *kets* or *ket vectors* and denoted by $|a\rangle$. Linear functionals Γ_b in the dual linear space V' are called *bras* or *bra vectors* and are denoted by $\langle b|$.

There is a one-to-one correspondence between kets in V and bras in V' or between vectors and linear functionals. We will use the *same label* to denote these corresponding quantities

$$|a\rangle \leftrightarrow \langle a| \tag{2.46}$$

The inner product between two vectors $|a\rangle$ and $|b\rangle$ in V corresponds to the linear functional of the left-hand vector assigning a scalar value to the right-hand vector

$$\Gamma_a(b) = (a, b) = \langle a \,|\, b\rangle = \text{ complex number} \tag{2.47}$$

The orthonormality property of a basis set $\{\alpha_i\}$ is expressed by the linear functional relation

$$\langle \alpha_i \,|\, \alpha_j \rangle = \delta_{ij} \tag{2.48}$$

The expansion of an arbitrary state in an orthonormal basis is given by

$$|q\rangle = \sum_n a_n \, |\alpha_n\rangle \tag{2.49}$$

and the expansion coefficients are

$$\langle \alpha_m \,|\, q \rangle = \sum_n a_n \, \langle \alpha_m \,|\, \alpha_n \rangle = \sum_n a_n \delta_{mn} = a_m \tag{2.50}$$

or a_m is the linear functional $\Gamma_{\alpha_m}(q)$ of the state $|q\rangle$ with respect to the corresponding basis vector $|\alpha_m\rangle$.

If we have two vectors $|a\rangle$ and $|b\rangle$ and we expand them in an orthonormal basis set $\{\alpha_i\}$ as

$$|a\rangle = \sum_n a_n |\alpha_n\rangle \text{ and } |b\rangle = \sum_n b_n |\alpha_n\rangle \tag{2.51}$$

$$\rightarrow \langle a \,|\, b\rangle = \sum_n a_n^* b_n = \langle b \,|\, a\rangle^* = \left(\sum_n b_n^* a_n\right)^* \tag{2.52}$$

where we have used the antilinear property of inner products that says that we have the correspondence

$$c\,|a\rangle \leftrightarrow c^*\,\langle a| \tag{2.53}$$

The linear functional itself is directly represented by the bra vector, i.e.,

$$\langle q|\cdots = \Gamma_q(\cdots) = (q, \cdots) \tag{2.54}$$

In Dirac language, there is nothing to distinguish between the value of the linear functional $\langle q|$ for the vector $|p\rangle$ and the inner product of the vectors $|q\rangle$ and $|p\rangle$. They are both $\langle q \,|\, p\rangle$. 2.7 **Gram-Schmidt Orthogonalization Process**

An orthonormal basis set for an n-dimensional vector space can always be constructed from any set of n linearly independent vectors using the Gram-Schmidt orthogonalization method.

Suppose that we have a set of n linearly independent vectors $|\alpha_i\rangle\,, i = 1, 2, \ldots, n$ that are not a mutually orthonormal set. We can construct a mutually orthonormal set $|\beta_i\rangle\,, i = 1, 2, \ldots, n$ using the following steps:

1. let

$$|\beta_1\rangle = |\alpha_1\rangle$$

2. let

   $|\beta_2\rangle = |\alpha_2\rangle + a_1 |\beta_1\rangle$ where we choose a_1 such that $\langle \beta_1 | \beta_2 \rangle = 0$

3. this gives

$$\langle \beta_1 | \beta_2 \rangle = 0 = \langle \beta_1 | \alpha_2 \rangle + a_1 \langle \beta_1 | \beta_1 \rangle$$

$$a_1 = -\frac{\langle \beta_1 | \alpha_2 \rangle}{\langle \beta_1 | \beta_1 \rangle}$$

Now proceed by induction.

Suppose we have constructed k mutually orthogonal vectors $|\beta_i\rangle, i = 1, 2, \ldots, k$. If we let

$$|\beta_{k+1}\rangle = |\alpha_{k+1}\rangle + \sum_{j=1}^{k} a_j |\beta_j\rangle \tag{2.55}$$

with

$$a_j = -\frac{\langle \beta_j \,|\, \alpha_{k+1} \rangle}{\langle \beta_j \,|\, \beta j \rangle} \tag{2.56}$$

then we have $\langle \beta_j \,|\, \beta_{k+1} \rangle = 0$ for $j = 1, 2, \ldots, k$. These steps are repeated until we have n mutually orthogonal vectors. We then normalize them to 1 and create an orthonormal set.

For example, suppose we have the set

$$|\alpha_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad |\alpha_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \qquad |\alpha_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \tag{2.57}$$

These vectors are not orthonormal.

1. let

$$|\beta_1\rangle = |\alpha_1\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \qquad \langle\beta_1 \,|\, \beta_1\rangle = 2$$

2. let

$$|\beta_2\rangle = |\alpha_2\rangle + a_1 \,|\beta_1\rangle$$

with

$$a_1 = -\frac{\langle\beta_1 \,|\, \alpha_2\rangle}{\langle\beta_1 \,|\, \beta_1\rangle} = -\frac{1}{2}$$

and thus

$$|\beta_2\rangle = |\alpha_2\rangle - \frac{1}{2}\,|\alpha_1\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix} \qquad \langle\beta_2 \,|\, \beta_2\rangle = \frac{3}{2} \qquad \langle\beta_1 \,|\, \beta_2\rangle = 0$$

3. let

$$|\beta_3\rangle = |\alpha_3\rangle + a_1\,|\beta_1\rangle + a_2\,|\beta_2\rangle$$

with

$$a_1 = -\frac{\langle\beta_1\,|\,\alpha_3\rangle}{\langle\beta_1\,|\,\beta_1\rangle} = -\frac{1}{2} \qquad a_2 = -\frac{\langle\beta_2\,|\,\alpha_3\rangle}{\langle\beta_2\,|\,\beta_2\rangle} = -\frac{1}{3}$$

and thus

$$|\beta_3\rangle = \frac{2}{3}\begin{pmatrix}1\\-1\\1\end{pmatrix} \qquad \langle\beta_3\,|\,\beta_3\rangle = \frac{4}{3} \qquad \langle\beta_1\,|\,\beta_3\rangle = 0 \qquad \langle\beta_2\,|\,\beta_3\rangle = 0$$

We normalize the vectors by dividing by their respective *norms*,

$$|\gamma_i\rangle = \frac{|\beta_i\rangle}{\|\,|\beta_i\rangle\,\|} = \frac{|\beta_i\rangle}{|\,\langle\beta_i\,|\,\beta_i\rangle\,|^{1/2}}$$

The orthonormal set is then

$$|\gamma_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix} \qquad |\gamma_2\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix}-1\\1\\2\end{pmatrix} \qquad |\gamma_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

2.8 **Linear Operators**

In general, an *operator* defined on a vector space maps vectors into vectors $\hat{Q} : V \to V$, i.e., if $\hat{Q}$ = operator and $|k\rangle$ = a vector, then $\hat{Q}\,|k\rangle = |q\rangle$ = a vector(we will use the $\hat{}$ symbol on top to signify operators). We say that $|q\rangle$ is the image of $|k\rangle$ under the mapping $\hat{Q}$. An operator is fully defined if we specify its action on all vectors in its *domain*, which is the set of all vectors for which $\hat{Q}\,|k\rangle$ for all $|k\rangle$ is defined. Its *range* is the set of all vectors of the form $\hat{Q}\,|k\rangle$ for all $|k\rangle$.

In the special case of a *linear operator*, the operator also satisfies the *linearity relation*

$$\hat{Q}(a_1\,|k_1\rangle + a_2\,|k_2\rangle) = \hat{Q}(a_1\,|k_1\rangle) + \hat{Q}(a_2\,|k_2\rangle) \tag{2.58}$$

In general, the operator $\hat{A}$ is linear if, for all $|f\rangle, |g\rangle \in V$, $\hat{A}(|f\rangle + |g\rangle) = \hat{A}|f\rangle + \hat{A}|g\rangle$, $(\alpha\hat{A})|f\rangle = (\alpha\hat{A}|f\rangle$ and $\hat{A} = 0$ if and only if $\hat{A}|f\rangle = 0$ for all $|f\rangle$. The *norm* $\|\hat{A}\|$ of the linear operator $\hat{A}$ is defined as the maximum of $\|\hat{A}|f\rangle\|$ for all $|f\rangle$ such that $\||f\rangle\| \leq 1$. The identity operator $\hat{I}$ is defined by $\hat{I}|f\rangle = |f\rangle$ for all $|f\rangle$.

Since any vector in the space can be written as a linear combination of a basis set of vectors, we need only define a linear operator on the basis set and then its operation on all vectors is known.

Quantum mechanics works exclusively with linear operators so we will just call them operators from now on.

When are two operators equal?

In general, we say that two operators are *equal*, i.e., $\hat{Q}_1 = \hat{Q}_2$, when $\hat{Q}_1|p\rangle = \hat{Q}_2|p\rangle$ for *all* vectors $|p\rangle$ in the intersection of the domains of $\hat{Q}_1$ and $\hat{Q}_2$.

Using this equality idea we can define the sum and product of operators by

$$(\hat{Q}_1 + \hat{Q}_2)\,|k\rangle = \hat{Q}_1\,|k\rangle + \hat{Q}_2\,|k\rangle \tag{2.59}$$

$$(\hat{Q}_1\hat{Q}_2)\,|k\rangle = \hat{Q}_1(\hat{Q}_2\,|k\rangle) \tag{2.60}$$

for all vectors $|k\rangle$. It is clear that these relations imply that

$$(\hat{Q}_1\hat{Q}_2\hat{Q}_3)\,|k\rangle = (\hat{Q}_1\hat{Q}_2)\hat{Q}_3\,|k\rangle = \hat{Q}_1(\hat{Q}_2\hat{Q}_3)\,|k\rangle \tag{2.61}$$

or

$$(\hat{Q}_1\hat{Q}_2)\hat{Q}_3 = \hat{Q}_1(\hat{Q}_2\hat{Q}_3) \tag{2.62}$$

which corresponds to *associativity*. Now

$$(\hat{Q}_1\hat{Q}_2)\,|k\rangle = \hat{Q}_1(\hat{Q}_2)\,|k\rangle) = \hat{Q}_1\,|k_2\rangle = |k_{12}\rangle \tag{2.63}$$

$$(\hat{Q}_2\hat{Q}_1)\,|k\rangle = \hat{Q}_2(\hat{Q}_1)\,|k\rangle) = \hat{Q}_2\,|k_1\rangle = |k_{21}\rangle \tag{2.64}$$

does not imply that $|k_{12}\rangle = |k_{21}\rangle$.

Therefore, in general we have $\hat{Q}_1\hat{Q}_2 = \hat{Q}_2\hat{Q}_1$, which corresponds to the *noncommutivity* of the two operators.

We define the *commutator* of two operators by

$$[\hat{Q}_1, \hat{Q}_2] = \hat{Q}_1\hat{Q}_2 - \hat{Q}_2\hat{Q}_1 \tag{2.65}$$

Two operators are said to *commute* if their corresponding commutator is zero (the null vector).

The commutator will be a fundamental quantity in our discussions of quantum mechanics.

2.9 **An Aside : The Connection to Matrices**

Now suppose that we have an N-dimensional vector space and we choose an orthonormal basis set

$$\{|q_i\rangle\, , i = 1, 2, \ldots, N\} \tag{2.66}$$

In an N-dimensional space, we can always represent any vector as an N-element column of numbers or as a column vector.

If we expand some arbitrary state $|\alpha\rangle$ in terms of this basis set and operate on it with an operator $\hat{Q}$, then we have

$$|\beta\rangle = \hat{Q}\,|\alpha\rangle = \hat{Q}\sum_{i=1}^{N} c_i\,|q_i\rangle = \sum_{i=1}^{N} c_i \hat{Q}\,|q_i\rangle \tag{2.67}$$

where $|\beta\rangle$ is another vector in the same space since $\hat{Q}$ is a linear operator.

Now expanding the vector $|\beta\rangle$ in the same basis set as

$$|\beta\rangle = \sum_{i=1}^{N} d_i\,|q_i\rangle \tag{2.68}$$

and constructing the linear functional(inner product) of $|\beta\rangle = \hat{Q}\,|\alpha\rangle$ with respect to $|q_i\rangle$ we get

$$\langle q_k|\,\hat{Q}\,|\alpha\rangle = \langle q_k|\,\hat{Q}\sum_{i=1}^{N} c_i\,|q_i\rangle = \sum_{i=1}^{N} c_i\,\langle q_k|\,\hat{Q}\,|q_i\rangle$$

$$= \langle q_k\,|\,\beta\rangle = \sum_{j=1}^{N} d_j\,\langle q_k\,|\,q_j\rangle \tag{2.69}$$

Using the orthonormality property of the basis set

$$\langle q_k\,|\,q_j\rangle = \delta_{kj} \tag{2.70}$$

we get

$$\langle q_k|\,\hat{Q}\,|q_i\rangle = \sum_{j=1}^{N} d_j\delta_{kj} = d_k \tag{2.71}$$

If we define the numbers $\hat{Q}_{ki} = \langle q_k|\,\hat{Q}\,|q_i\rangle$ we get the relation

$$\sum_{j=1}^{N} \hat{Q}_{ki}c_i = d_k \tag{2.72}$$

Clearly, this has the form of a matrix equation where $\hat{Q}_{ki} = \langle q_k | \hat{Q} | q_i \rangle$ is defined as the (ki)-matrix element of the operator $\hat{Q}$. In this case, we would have the representation

$$(\hat{Q}_{ij}) = N \times N \text{ matrix} \tag{2.73}$$

$$(c_i) = N \times 1 \text{ column matrix} \tag{2.74}$$

$$(d_i) = N \times 1 \text{ column matrix} \tag{2.75}$$

and the matrix equation (using matrix multiplication) represented above is $Qc = d$.

All finite dimensional vector space operator equations can be turned into matrix equations in this manner.

2.10 **More about Vectors, Linear Functionals, Operators**

We have discussed what happens when an operator acts to the right on a ket vector. What about acting to the left on a bra vector, i.e., what is the meaning of the quantity

$$\langle q|\,\hat{Q} \tag{2.76}$$

Since the bra vector is really a linear functional we must be careful and look very closely at the mathematical content of the above quantity. Remember that the definition of the linear functional was

$$\langle q\,|\,p\rangle = \Gamma_q(p) = (q,p) \tag{2.77}$$

The standard *definition* (in terms of inner products) of the *adjoint* operator $\hat{Q}^\dagger$, of the operator $\hat{Q}$, in a linear vector space is

$$(\hat{Q}^\dagger q, p) = (q, \hat{Q}p) \tag{2.78}$$

The adjoint obeys the following properties:

$$\|\hat{A}^\dagger\| = \|\hat{A}\| \qquad (\hat{A}^\dagger)^\dagger = \hat{A} \qquad (\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger \tag{2.79}$$

$$(\alpha\hat{A})^\dagger = \alpha^*\hat{A}^\dagger \qquad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger \qquad (\hat{A}^{-1})^\dagger = (\hat{A}^\dagger)^{-1} \tag{2.80}$$

If we define a new vector ϕ by the operation $\hat{Q}^\dagger q = \phi$, then using the definition of the adjoint operator we have

$$\Gamma_\phi(p) = (\phi, p) = (\hat{Q}^\dagger q, p) = (q, \hat{Q}p) = \Gamma_q(\hat{Q}p) \tag{2.81}$$

We want the action of an operator on the bra space of linear functionals or bra vectors to create a new linear functional or bra vector in the same way that it does for ket vectors. We can guarantee this by *defining* the operation of an operator on the bra space of linear functionals by

$$\hat{Q}\Gamma_q(p) = \Gamma_q(\hat{Q}p) \tag{2.82}$$

Using this new definition and the definition of a linear functional, we then have

$$\hat{Q}\Gamma_q(c_1p_1 + c_2p_2) = \Gamma_q(\hat{Q}(c_1p_1 + c_2p_2)) \tag{2.83}$$

$$= c_1\Gamma_q(\hat{Q}p_1) + c_2\Gamma_q(\hat{Q}p_2) \tag{2.84}$$

$$= c_1\hat{Q}\Gamma_q(p_1) + c_2\hat{Q}\Gamma_q(p_2) \tag{2.85}$$

which says that $\hat{Q}\Gamma_q(\ldots)$ itself is also a linear functional.

Thus, our definition of how an operator acts on the bra space of linear functionals simply says that it creates a new functional as we desired.

With this definition, we then have

$$\hat{Q}\Gamma_q(p) = \Gamma_\phi(p) = (\phi, p) = (\hat{Q}^\dagger q, p) = (q, \hat{Q}p) = \Gamma_q(\hat{Q}p) \tag{2.86}$$

or, since $(\hat{Q}^\dagger q, p) = \Gamma_{\hat{Q}^\dagger q}(p)$, the relationship among linear functionals is

$$\hat{Q}\Gamma_q(\ldots) = \Gamma_{\hat{Q}^\dagger q}(p) \tag{2.87}$$

In terms of bra and ket vectors, this says that if $\langle q|$ and $|q\rangle$ are *corresponding* bra and ket vectors(remember, the Riesz theorem says there is a unique bra vector for each ket vector), then

$$\hat{Q}\,|q\rangle = |\beta\rangle \quad \text{and} \quad \langle q|\,\hat{Q}^\dagger = \langle\beta| \tag{2.88}$$

should also be emphcorresponding bra and ket vectors.

Since $\langle\beta\,|\,p\rangle^* = \langle p\,|\,\beta\rangle$ we then have that

$$\langle q|\,\hat{Q}^\dagger\,|p\rangle^* = \langle p|\,\hat{Q}\,|q\rangle \tag{2.89}$$

for all p and q. This relation is *equivalent* to the original inner product relation

$$(\hat{Q}^\dagger q, p) = (q, \hat{Q}p) \tag{2.90}$$

The *end result* of this discussion is that $\langle q|\,\hat{Q}^\dagger = \langle \beta|$ is the bra vector(linear functional) corresponding to the ket vector $\hat{Q}\,|q\rangle = |\beta\rangle$. Since the adjoint operator satisfies the relations

$$(c\hat{Q})^\dagger = c^*\hat{Q}^\dagger \qquad (\hat{Q}\hat{R})^\dagger = \hat{R}^\dagger\hat{Q}^\dagger \qquad (\hat{Q}+\hat{R})^\dagger = \hat{Q}^\dagger + \hat{R}^\dagger \quad (2.91)$$

we can define another product among the bra and ket vectors, which is an operator rather than a scalar as in the case of the inner product. It is called the *outer product* and, in the Dirac language, has the form

$$|q\rangle\,\langle p| \quad (2.92)$$

It is clear that the outer product is an operator since its action on any other vector always results in a vector

$$(|q\rangle\,\langle p|)\,|s\rangle = |q\rangle\,\langle p\,|\,s\rangle \quad (2.93)$$

We also have that

$$(\langle q|\,(|q\rangle\,\langle p|)^\dagger\,|p\rangle)^* = \langle p|\,(|q\rangle\,\langle p|)\,|q\rangle = \langle p\,|\,q\rangle\,\langle p\,|\,q\rangle = (\langle q\,|\,p\rangle\,\langle q\,|\,p\rangle)^* \quad (2.94)$$

or

$$(\langle q| \left(|q\rangle \langle p|\right)^\dagger |p\rangle) = \langle p \,|\, q\rangle \langle p \,|\, q\rangle \tag{2.95}$$

which implies that

$$\left(|q\rangle \langle p|\right)^\dagger = |q\rangle \langle p| \tag{2.96}$$

This type of operator will be very important in our later discussions. The special case

$$|p\rangle \langle p| \tag{2.97}$$

is called a *projection operator* because it picks out the component of an arbitrary state vector in the *"direction"* of the vector $|p\rangle$.

Projections operators (and linear combinations) will be the mathematical object with a direct connection to physical states and measurements in our later discussions.

Example in a Finite Dimensional Vector Space

Let us consider the 2-dimensional vector space spanned by the orthonormal basis set

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2.98}$$

We can define two projection operators as

$$\hat{P}_1 = |1\rangle \langle 1| \qquad \hat{P}_2 = |2\rangle \langle 2| \tag{2.99}$$

The matrix representation of these two projection operator is easily found using $\langle 1 \,|\, 1\rangle = \langle 2 \,|\, 2\rangle = 1$ and $\langle 1 \,|\, 2\rangle = \langle 2 \,|\, 1\rangle = 0$ and $\hat{Q}_{ki} = \langle k| \hat{Q} |i\rangle$. We have

$$(\hat{P}_1) = \begin{pmatrix} \langle 1|\,\hat{P}_1\,|1\rangle & \langle 1|\,\hat{P}_1\,|2\rangle \\ \langle 2|\,\hat{P}_1\,|1\rangle & \langle 2|\,\hat{P}_1\,|2\rangle \end{pmatrix}$$
$$= \begin{pmatrix} \langle 1\,|\,1\rangle\langle 1\,|\,1\rangle & \langle 1\,|\,1\rangle\langle 1\,|\,2\rangle \\ \langle 2\,|\,1\rangle\langle 1\,|\,1\rangle & \langle 2\,|\,1\rangle\langle 1\,|\,2\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.100}$$

$$(\hat{P}_2) = \begin{pmatrix} \langle 1|\,\hat{P}_2\,|1\rangle & \langle 1|\,\hat{P}_2\,|2\rangle \\ \langle 2|\,\hat{P}_2\,|1\rangle & \langle 2|\,\hat{P}_2\,|2\rangle \end{pmatrix}$$
$$= \begin{pmatrix} \langle 1\,|\,2\rangle\langle 2\,|\,1\rangle & \langle 1\,|\,2\rangle\langle 2\,|\,2\rangle \\ \langle 2\,|\,2\rangle\langle 2\,|\,1\rangle & \langle 2\,|\,2\rangle\langle 2\,|\,2\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.101}$$

Now consider an arbitrary vector in this space

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1\,|1\rangle + a_2\,|2\rangle \tag{2.102}$$

We then have (using both Dirac and matrix languages)

$$\hat{P}_1 \left|a\right\rangle = a_1 \left|1\right\rangle \left\langle 1 \,\middle|\, 1\right\rangle + a_2 \left|1\right\rangle \left\langle 1 \,\middle|\, 2\right\rangle = a_1 \left|1\right\rangle \tag{2.103}$$

or

$$(\hat{P}_1) \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} a_1 \\ 0 \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.104}$$

and the projection operator performs as advertised.

We note that (at least in this *special case*)

$$\begin{aligned} (\hat{P}_1) + (\hat{P}_2) &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \hat{I} = \text{identity operator} \end{aligned} \tag{2.105}$$

or

$$\begin{aligned} (\hat{P}_1) + (\hat{P}_2) \left|a\right\rangle &= \left(\left\langle 1 \,\middle|\, 1\right\rangle + \left\langle 2 \,\middle|\, 2\right\rangle\right) \left|a\right\rangle \\ &= \sum_{j=1}^{2} \left|j\right\rangle \left\langle j \,\middle|\, a\right\rangle = \left|a\right\rangle = \hat{I} \left|a\right\rangle \end{aligned} \tag{2.106}$$

where we have made use of the expansion formula for an arbitrary state in an orthonormal basis.

Return to Gram-Schmidt

As before, suppose we have a set of linearly independent, but non-orthogonal vectors $|i\rangle$ in an n-dimensional linear vector space, we can construct a set of orthogonal vectors $|\alpha_i\rangle$ as follows:

$$|\alpha_1\rangle = |1\rangle \qquad |\alpha_2\rangle = |2\rangle - |\alpha_1\rangle \langle\alpha_1 \,|\, 2\rangle \tag{2.107}$$

where

$$|\alpha_1\rangle \langle\alpha_1| = \hat{P}_{\alpha_1} = \text{ projection operator} \tag{2.108}$$

Then

$$|\alpha_2\rangle = |2\rangle - \hat{P}_{\alpha_1} |2\rangle \tag{2.109}$$

As earlier, the fact that this type of operator is a *projection operator* is shown clearly by considering its effect on an arbitrary vector

$$|Q\rangle = q_1 |1\rangle + q_2 |2\rangle + q_3 |3\rangle + \ldots = \sum_i q_i |i\rangle \tag{2.110}$$

Then using

$$\hat{P}_{\alpha_n} = |\alpha_n\rangle \langle\alpha_n| \tag{2.111}$$

we get

$$\hat{P}_{\alpha_n} |Q\rangle = \sum_i q_i \hat{P}_{\alpha_n} |i\rangle = \sum_i q_i |\alpha_n\rangle \langle\alpha_n \,|\, i\rangle = \sum_i q_i |\alpha_n\rangle \delta_{ni} = q_n |\alpha_n\rangle \tag{2.112}$$

or

$$\sum_n |\alpha_n\rangle \langle\alpha_n| = \hat{I} = \text{ identity operator} \tag{2.113}$$

which makes perfect sense since if you project out all components of a vector you just get the vector back! This generalizes the earlier result we found in the 2-dimensional space.

This Dirac language is very interesting!

We can then write a general Gram-Schmidt procedure as

$$|\alpha_1\rangle = |1\rangle \qquad |\alpha_2\rangle = (1 - \hat{P}_{\alpha_1})\,|2\rangle \qquad |\alpha_3\rangle = (1 - \hat{P}_{\alpha_1} - \hat{P}_{\alpha_2})\,|3\rangle$$

$$\cdots\cdots\cdots\cdots\cdots$$

$$|\alpha_n\rangle = \left(1 - \sum_{k=1}^{n-1} \hat{P}_{\alpha_k}\right)|n\rangle$$

which is rather neat. *This shows the power of these projection operators and of the Dirac language.*

Important Point - Looking at the equations

$$\hat{Q}\,|q\rangle = |\beta\rangle \quad \textit{and} \quad \langle q|\,\hat{Q}^{\dagger} = \langle\beta| \tag{2.114}$$

we might be tempted(as is the case in many textbooks) at this point to write

$$(|q\rangle)^\dagger = \langle q| \tag{2.115}$$

This might seem to make sense in a finite dimensional vector space where we can always treat kets as *column vectors* and bras as *row vectors*. However, the adjoint symbol is really only defined for operators and not for vectors, so one should exercise great care before generalizing this result, especially in infinite dimensional spaces!

Finally, we define a property of an operator called the *trace* as

$$Tr\hat{Q} = \sum_j \langle q_j| \hat{Q} |q_j\rangle = \text{ sum of diagonal elements } = \sum_j (\hat{Q})_{jj} \tag{2.116}$$

2.11 **Self-Adjoint Operators**

If we have an operator $\hat{Q}$ where the adjoint satisfies the relation

$$\langle q| \hat{Q}^\dagger |p\rangle = (\langle p| \hat{Q} |q\rangle)^* \tag{2.117}$$

then $\hat{Q}$ is a *Hermitian* or *self-adjoint* operator.

In a finite-dimensional space, we can look at the matrix elements corresponding to a Hermitian operator. Let

$$|p\rangle = \sum_{i=1}^{N} a_i |q_i\rangle \tag{2.118}$$

We have

$$\langle q_k| \hat{Q} |p\rangle^* = \langle p| \hat{Q} |q_k\rangle \tag{2.119}$$

$$\langle q_k| \hat{Q} \sum_{i=1}^{N} a_i \, |q_i\rangle^* = \sum_{i=1}^{N} a_i^* \, \langle q_i| \hat{Q} \, |q_k\rangle \tag{2.120}$$

$$\sum_{i=1}^{N} a_i^* \, \langle q_k| \hat{Q} \, |q_i\rangle = \sum_{i=1}^{N} a_i^* \, \langle q_i| \hat{Q} \, |q_k\rangle \tag{2.121}$$

$$\sum_{i=1}^{N} a_i^* [\langle q_k| \hat{Q} \, |q_i\rangle^* - \langle q_i| \hat{Q} \, |q_k\rangle] = 0 \tag{2.122}$$

where we have used the *antilinear* property.

This says that the matrix elements of a Hermitian operator satisfy

$$\hat{Q}_{ki}^* = \hat{Q}_{ik} \qquad or \qquad \hat{Q}^\dagger = \hat{Q} \tag{2.123}$$

as we saw above.

If $\hat{H}, \hat{K}$ are Hermitian, then so are $\hat{H} + \hat{K}$, $i[\hat{H}, \hat{K}]$, and $\alpha\hat{H}$ for all real α, and $\hat{A}^\dagger \hat{H} \hat{A}$ for any operator $\hat{A}$, but $\hat{H}\hat{K}$ is Hermitian if and only if the commutator $[\hat{H}, \hat{K}] = 0$.

The Hermitian operator $\hat{H}$ is positive if $(f, \hat{H}f) = \langle f | \hat{H} | f \rangle \geq 0$ for all $|f\rangle$; note that if the equality holds for all $|f\rangle$, then $\hat{H} = 0$. If $\hat{H}$ is positive, then it obeys the inequality

$$|(f, \hat{H}g)|^2 \leq (f, \hat{H}f)(g, \hat{H}g) \tag{2.124}$$

called the *Schwarz inequality for positive operators*.

If $\hat{K}^\dagger = -\hat{K}$, then the operator $\hat{K}$ is called *antihermitian*; clearly, $i\hat{K}$ is Hermitian. An arbitrary operator $\hat{A}$ can always be written as the sum $\hat{A} = \hat{H}_A + \hat{K}_A$ of its Hermitian part

$$\hat{H}_A = \frac{1}{2}(\hat{A} + \hat{A}^\dagger) \tag{2.125}$$

and its antihermitian part

$$\hat{K}_A = \frac{1}{2}(\hat{A} - \hat{A}^\dagger) \tag{2.126}$$

Hermitian operators will be very important in our discussions because they will represent *measurable quantities or observables.*

2.12 **Eigenvalues and Eigenvectors**

Suppose that an operator $\hat{Q}$ acting on a particular vector $|\beta\rangle$ returns a scalar multiple of that vector

$$\hat{Q}\,|\beta\rangle = b\,|\beta\rangle \tag{2.127}$$

The vector $|\beta\rangle$ is then called an *eigenvector* and the scalar b an *eigenvalue* of the operator $\hat{Q}$. Using the definition of the adjoint $\hat{Q}^\dagger$ operator and the antilinear correspondence between bras and kets, we then also must have (using any arbitrary vector $|\alpha\rangle$)

$$\langle\alpha|\,\hat{Q}\,|\beta\rangle^* = b^*\,\langle\alpha\,|\,\beta\rangle^* \tag{2.128}$$

$$\langle\beta|\,\hat{Q}^\dagger\,|\alpha\rangle = b^*\,\langle\beta\,|\,\alpha\rangle \tag{2.129}$$

$$\langle\beta|\,\hat{Q}^\dagger = b^*\,\langle\beta| \tag{2.130}$$

Now we assume that $\hat{Q}$ is a Hermitian operator and that $\hat{Q}\,|\beta\rangle = b\,|\beta\rangle$ again. The Hermitian property says that

$$\langle\beta|\,\hat{Q}^{\dagger}\,|\beta\rangle = \langle\beta|\,\hat{Q}\,|\beta\rangle = \langle\beta|\,\hat{Q}\,|\beta\rangle^{*} \tag{2.131}$$

$$\langle\beta|\,b\,|\beta\rangle = \langle\beta|\,b\,|\beta\rangle^{*} \tag{2.132}$$

$$(b - b^{*})\,\langle\beta\,|\,\beta\rangle = 0 \tag{2.133}$$

$$b = b^{*} \tag{2.134}$$

where we have assumed that $\langle\beta\,|\,\beta\rangle \neq 0$. This means that all of the eigenvalues of a Hermitian operator are *real*. Following this up, if $\hat{Q}$ is a Hermitian operator which satisfies

$$\hat{Q}\,|\beta\rangle = b\,|\beta\rangle \quad with \quad \hat{Q} = \hat{Q}^{\dagger} \tag{2.135}$$

then

$$\langle\beta|\,\hat{Q} = b\,\langle\beta| \tag{2.136}$$

or the ket vector and its corresponding bra vector are eigenvectors with the *same* eigenvalue.

Suppose that we have two eigenvectors $|\alpha\rangle$ and $|\beta\rangle$ of a Hermitian operator $\hat{Q}$ with eigenvalues a and b, respectively. We then have

$$\hat{Q}\,|\alpha\rangle = a\,|\alpha\rangle \quad \textit{and} \quad \hat{Q}\,|\beta\rangle = b\,|\beta\rangle \tag{2.137}$$

$$0 = \langle\alpha|\,\hat{Q}\,|\beta\rangle - \langle\beta|\,\hat{Q}^{\dagger}\,|\alpha\rangle^{*} = \langle\alpha|\,\hat{Q}\,|\beta\rangle - \langle\beta|\,\hat{Q}\,|\alpha\rangle^{*} \tag{2.138}$$

$$0 = b\,\langle\alpha\,|\,\beta\rangle - a^{*}\,\langle\beta\,|\,\alpha\rangle^{*} = (b-a)\,\langle\alpha\,|\,\beta\rangle \tag{2.139}$$

This implies that eigenvectors corresponding to *distinct(different)* eigenvalues ($a \neq b$) are *orthogonal*, i.e., $\langle\alpha\,|\,\beta\rangle = 0$.

If $a = b$, that is, the two eigenvectors correspond to the same eigenvalue, then they are called *degenerate* eigenvectors. In this case, we have that

$$\hat{Q}\,|\alpha\rangle = a\,|\alpha\rangle \quad \textit{and} \quad \hat{Q}\,|\beta\rangle = a\,|\beta\rangle \tag{2.140}$$

Now, any linear combination of the degenerate eigenvectors is also an eigenvector with the same eigenvalue as can be seen below

$$\begin{aligned}\hat{Q}(c_1 |\alpha\rangle + c_2 |\beta\rangle) &= c_1\hat{Q} |\alpha\rangle + c_2\hat{Q} |\beta\rangle \\ &= c_1 a |\alpha\rangle + c_2 a |\beta\rangle = a(c_1 |\alpha\rangle + c_2 |\beta\rangle)\end{aligned} \tag{2.141}$$

It is, therefore, always possible to replace a nonorthogonal but linearly independent set of degenerate eigenvectors by linear combinations of themselves that are orthogonal (using the Gram-Schmidt process). For the case of two states above, the orthogonal set is easy to find, namely

$$|1\rangle = |\alpha\rangle + |\beta\rangle \qquad |2\rangle = |\alpha\rangle - |\beta\rangle \tag{2.142}$$

The number of distinct vectors corresponding to a given eigenvalue is called the *multiplicity* of that eigenvalue. Non-degenerate eigenvalues are called *simple*.

We will always assume that we have already carried out this orthogonalization process and that the set of eigenvectors(for both non-degenerate and degenerate eigenvalues) of any Hermitian operator is an orthogonal set.

If the norms are all finite, then we can always construct an *orthonormal* set where

$$\langle \alpha_i \,|\, \alpha_j \rangle = \delta_{ij} \tag{2.143}$$

The set of eigenvalues of an operator $\hat{A}$ is called the *spectrum* of $\hat{A}$.

In an m-dimensional space $\mathcal{H}$ choose a matrix representation in which $\hat{A} = (A_{ij}), g = (\gamma_i)$. Written in this representation, the eigenvalue equation $\hat{A}g = \lambda g$ becomes a system of m homogeneous linear equations in the γ_i. The eigenvalues λ are the roots of the algebraic equation of degree m

$$det(A_{ij} - \lambda\delta_{ij}) = 0 \tag{2.144}$$

known as the *secular equation*, which expresses the condition for the homogeneous system of equations to have non-trivial solutions. In an m-dimensional space every operator has at least one and at most m distinct eigenvalues. If all the eigenvalues of an arbitrary operator $\hat{A}$ are simple, then there are m linearly independent eigenvectors of $\hat{A}$ but there may be fewer if $\hat{A}$ has multiple eigenvalues.

2.13 **Completeness**

A set of orthonormal vectors $\{|\alpha_k\rangle, k = 1, 2, 3, \ldots, N\}$ is *complete* if we can expand an arbitrary vector $|\eta\rangle$ in terms of that set, i.e.,

$$|\eta\rangle = \sum_j a_j |\alpha_j\rangle \tag{2.145}$$

The orthonormality condition then allows us to calculate the expansion coefficients a_j as

$$\langle\alpha_k | \eta\rangle = \sum_j a_j \langle\alpha_k | \alpha_j\rangle = \sum_j a_j \delta_{kj} = a_k \tag{2.146}$$

This implies that(remember the 2-dimensional example earlier)

$$|\eta\rangle = \sum_j |\alpha_j\rangle \langle\alpha_j | \eta\rangle = \left(\sum_j |\alpha_j\rangle \langle\alpha_j| \right) |\eta\rangle \tag{2.147}$$

or

$$\sum_j |\alpha_j\rangle \langle\alpha_j| = \hat{I} = \text{ identity operator} \tag{2.148}$$

This result is quite general.

For any complete set of vectors $\{|q_k\rangle, k = 1, 2, 3, \ldots, N\}$ the sum over all of the *projection* operators $|q_k\rangle \langle q_k|$ is the identity operator. This is one of the most important results we will derive. It will enable us to perform very clever tricks during algebraic manipulations. It is fundamentally linked to the probability interpretation of quantum mechanics as we shall see later.

If a set of vectors $\{|q_k\rangle, k = 1, 2, 3, \ldots, N\}$ are eigenvectors of a Hermitian operator $\hat{Q}$, then we will *always assume that they are a complete set.* Thus, if

$$\hat{Q}\,|q_k\rangle = q_k\,|q_k\rangle \tag{2.149}$$

then we can always write

$$\hat{Q} = \hat{Q}\hat{I} = \hat{Q}\sum_j |q_j\rangle\langle q_j| = \sum_j q_j\,|q_j\rangle\langle q_j| \tag{2.150}$$

which completely expresses an operator *in terms of its eigenvectors and eigenvalues.*

Since we can use the same argument to show that

$$\hat{Q}^n = \hat{Q}^n\hat{I} = \hat{Q}^n\sum_j |q_j\rangle\langle q_j| = \sum_j q_j^n\,|q_j\rangle\langle q_j| \tag{2.151}$$

we then have for any function $f(x)$ that has a power series expansion of the form

$$f(x) = \sum_k c_k x^k \tag{2.152}$$

that

$$\begin{aligned} f(\hat{Q}) = f(\hat{Q})\hat{I} = f(\hat{Q}) \sum_j |q_j\rangle \langle q_j| = \sum_j \sum_k c_k \hat{Q}^k |q_j\rangle \langle q_j| \\ = \sum_j \sum_k c_k q_j^k |q_j\rangle \langle q_j| = \sum_j f(q_j) |q_j\rangle \langle q_j| \end{aligned} \tag{2.153}$$

For a *finite dimensional space*, it can be shown that the eigenvectors of a Hermitian operator always form a complete set and all of the above relations hold. For infinite dimensional spaces the proof is not easily carried out in general (it is usually true however).

Before proceeding to a general discussion of the eigenvalue spectrum, the spectral theorem and the problem of continuous

eigenvalues let us expand our knowledge of some of the objects we have already defined and add a few definitions that will be useful.

2.14 **Expand Our Knowledge - Selected topics for the mathematically inclined.**

2.14.1 **Hilbert Space**

In an infinite dimensional space, we must determine whether the sums involved in many of our definitions *converge*. If they do not converge in some expressions, then the corresponding definitions are not valid. In addition, we must clearly state *what is meant* by a linear combination of an infinite number of vectors?

We assume that an *infinite linear combination*

$$|\alpha\rangle = \sum_{k=1}^{\infty} a_k \, |q_k\rangle \tag{2.154}$$

is *defined* if the sequence of partial sums

$$|\alpha_n\rangle = \sum_{k=1}^{n} a_k \, |q_k\rangle \tag{2.155}$$

converges as $n \to \infty$ or, equivalently, that $|\alpha_n\rangle \to |\alpha\rangle$ as $n \to \infty$, where this convergence is defined by the norm relation

$$\| \, |\alpha\rangle - |\alpha_n\rangle \, \| \to 0 \, as \, n \to \infty \tag{2.156}$$

The vector $|\alpha\rangle$ is called the *limit vector* of the sequence. A sequence of vectors $|\alpha_n\rangle$ is called a *Cauchy sequence* if

$$\| \, |\alpha_m\rangle - |\alpha_n\rangle \, \| \to 0 \, as \, m, n \to \infty \tag{2.157}$$

A space is *complete* if every Cauchy sequence of vectors converges to a limit vector in the space.

If a linear space with an inner product defined is complete, then it is called a *Hilbert space*.

A Hilbert space is *separable* if it has an orthonormal basis consisting of a countable (finite or infinite) number of vectors. Note that every finite-dimensional space is complete(as we assumed earlier).

If a set of n vectors $\{|q_k\rangle$ is such that every sequence of vectors in the set

$$|\alpha_n\rangle = \sum_{k=1}^{n} a_k \, |q_k\rangle \tag{2.158}$$

has a limit vector also in the set, then the set is *closed*.

Some examples are:

Space ℓ^2: this is the space of infinite sequences

$$(x_1, x_2, x_3, \ldots\ldots)$$

such that

$$\sum_{k=1}^{\infty} |x_k|^2 \; is \; finite$$

This space is a separable Hilbert space. It has an orthonormal basis consisting of

$$|q_1\rangle = (1,0,0,0,\ldots),\ |q_2\rangle = (0,1,0,0,\ldots),\ |q_3\rangle = (0,0,1,0,\ldots)\ \ldots$$

since

$$(x_1, x_2, x_3, \ldots\ldots) = \sum_{k=1}^{\infty} x_k \, |q_k\rangle$$

Space $\mathbf{L^2(a,b)}$: this is the space of square integrable functions on the interval (a,b). It is a separable Hilbert space. If we choose the interval $(0,1)$, then we have the space $L^2(0,1)$ of square integrable functions $f(x)$ on the interval $0 \leq x \leq 1$.

Another example comes from the theory of Fourier series, which says that the set of orthonormal vectors (or functions in this case)

$$1, \sqrt{2}\cos 2\pi kx \text{ and } \sin 2\pi kx \; for \; k = 1, 2, 3, \ldots$$

form an orthonormal basis.

If a set of vectors within a larger set is closed and both the larger set and the smaller set both form linear vector spaces, the smaller set is called a *subspace* of the larger set.

A subspace of a separable Hilbert space is also a separable Hilbert space.

If $\mathcal{R}$ is a subspace of a separable Hilbert space, then the set of all vectors which are *orthogonal to every vector* in $\mathcal{R}$ is called the *orthogonal complement* $\mathcal{R}_\perp$ of $\mathcal{R}$. $\mathcal{R}_\perp$is also a subspace.

A Hilbert space *preserves* the *one-to-one correspondence* between the kets in the space and the bras or linear functionals in its dual space.

2.14.2 **Bounded Operators**

A linear operator $\hat{Q}$ is *continuous* if

$$\hat{Q}\,|\alpha_n\rangle \to \hat{Q}\,|\alpha\rangle \tag{2.159}$$

for any sequence of vectors $|\alpha_n\rangle$ which converge to the limit vector $|\alpha\rangle$.

A linear operator is *bounded* if there exists a positive number a such that

$$\|\hat{Q}\,|\alpha\rangle\,\| \leq a\|\,|\alpha\rangle\,\| \tag{2.160}$$

for every vector $|\alpha\rangle$ in the space. The *smallest* a is called the *norm* $\|\hat{Q}\|$ of $\hat{Q}$.

A linear operator is continuous if and only if it is bounded. Every operator on a finite-dimensional space is bounded. A bounded linear operator on an infinite-dimensional space can be represented by an infinite matrix.

2.14.3 **Inverses**

A linear operator $\hat{Q}$ has an *inverse* if there exists a linear operator $\hat{M}$ such that

$$\hat{M}\hat{Q} = \hat{I} = \hat{Q}\hat{M} \tag{2.161}$$

We denote the inverse of $\hat{Q}$ by $\hat{M} = \hat{Q}^{-1}$.

In an n-dimensional vector space with a basis set $\{|q_k\rangle, k = 1, 2, 3, \ldots, n\}$, a necessary and sufficient condition for a linear operator $\hat{Q}$ to have an inverse is *any one* of the following (all are equivalent):

1. there is no vector $|\chi\rangle$ (except null vector) such that $\hat{Q}|\chi\rangle = 0$.

2. the set of vectors $\{\hat{Q}|q_k\rangle, k = 1, 2, 3, \ldots, n\}$ is linearly independent.

3. there exists a linear operator $\hat{M}$ such that $\hat{M}\hat{Q} = \hat{I} = \hat{Q}\hat{M}$

4. the matrix corresponding to $\hat{Q}$ has a nonzero determinant.

We defined the matrix elements with respect to a basis set by $\hat{Q}_{ij} = \langle q_i | \hat{Q} | q_j \rangle$. The determinant of a matrix is defined by

$$det(\hat{Q}) = \sum_{i_1 i_2 \ldots i_n} \epsilon_{i_1 i_2 \ldots i_n} \hat{Q}_{i_1 1} \hat{Q}_{i_2 2} \ldots \hat{Q}_{i_n n} \tag{2.162}$$

where $\epsilon_{i_1 i_2 \ldots i_n}$ is the permutation symbol of order n (n indices) which is defined by

$$\epsilon_{i_1 i_2 \ldots i_n} = \begin{cases} +1 & \text{if } i_1 i_2 \ldots i_n \text{ is an even permutation of } 123 \ldots n \\ -1 & \text{if } i_1 i_2 \ldots i_n \text{ is an odd permutation of } 123 \ldots n \\ 0 & \text{if any index is repeated} \end{cases} \tag{2.163}$$

Example: in the 3×3 case:

$$
\begin{aligned}
det \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{32} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} &= \sum_{i,j,k=1}^{3} \epsilon_{ijk} A_{i1} A_{j2} A_{k3} \\
&= \epsilon_{123} A_{11} A_{22} A_{33} + \epsilon_{132} A_{11} A_{32} A_{23} + \epsilon_{213} A_{21} A_{12} A_{33} \\
&\quad + \epsilon_{231} A_{21} A_{32} A_{13} + \epsilon_{312} A_{31} A_{12} A_{23} + \epsilon_{321} A_{31} A_{22} A_{13} \\
&= A_{11} A_{22} A_{33} - A_{11} A_{32} A_{23} - A_{21} A_{12} A_{33} \\
&\quad + A_{21} A_{32} A_{13} + A_{31} A_{12} A_{23} - A_{31} A_{22} A_{13}
\end{aligned}
$$

where we have only included the nonzero terms(no repeated indices).

We note that Rules (1), (2), (3) are *not sufficient conditions* in the infinite-dimensional case.

Finally, if two linear operators have inverses, then the inverse of their product is

$$(\hat{M}\hat{N})^{-1} = \hat{N}^{-1}\hat{M}^{-1} \tag{2.164}$$

2.14.4 **Unitary Operators**

A linear operator $\hat{G}$ is *unitary* (*orthogonal* if we have a real linear space) if it has an inverse and if $\|\hat{G}\,|\alpha\rangle\,\| = \|\,|\alpha\rangle\,\|$ for every vector $|\alpha\rangle$, i.e., unitary operators *preserve norms* or lengths of vectors.

If $\hat{G}$ is a unitary operator, then a more general result is

$$|\alpha_1\rangle = \hat{G}\,|\beta_1\rangle \quad \text{and} \quad |\alpha_2\rangle = \hat{G}\,|\beta_2\rangle \rightarrow \quad \langle\alpha_1\,|\,\alpha_2\rangle = \langle\beta_1\,|\,\beta_2\rangle \tag{2.165}$$

or unitary operators preserve inner products and not just norms. Using the fact that $\langle\alpha_1| = \langle\beta_1|\,\hat{G}$, we then have, for a unitary operator $\hat{G}$

$$\langle\alpha_1\,|\,\alpha_2\rangle = \langle\beta_1|\,\hat{G}^\dagger\hat{G}\,|\beta_2\rangle \;\text{ or }\; \hat{G}^\dagger\hat{G} = \hat{I} \;\text{ or }\; \hat{G}^\dagger = \hat{G}^{-1} \tag{2.166}$$

i.e., the inverse is the Hermitian conjugate or adjoint.

In addition, the action of a unitary operator on a basis set preserves the fact that it is a basis set.

The evolution of quantum systems in time will be given by a unitary operator. The inner product preserving property will be connected to the probability interpretation of quantum mechanics.

2.14.5 **More on Matrix Representations**

Let $\{|b_i\rangle\}$ be an orthonormal basis on an m-dimensional space. An arbitrary vector $|g\rangle$ can be written in terms of its components $\gamma_i = \langle b_i \,|\, g\rangle \,, i = 1, 2, \ldots, m$ as

$$|g\rangle = \sum_i \gamma_i \, |b_i\rangle \tag{2.167}$$

Given an operator $\hat{A}$, the vector $|h\rangle = \hat{A} \, |g\rangle$ has the components

$$\eta_i = \langle b_i | \left(\hat{A} \, |g\rangle \right) = \langle b_i | \, \hat{A} \, |g\rangle = \sum_i \gamma_j \, \langle b_i | \, \hat{A} \, |b_j\rangle \tag{2.168}$$

One can identify the vectors $|g\rangle$ and $|h\rangle$ with column matrices formed by their components

$$|g\rangle = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \dots \\ \gamma_m \end{pmatrix} \qquad |h\rangle = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_m \end{pmatrix} \tag{2.169}$$

In fact, the vector space of column matrices with the usual definitions of addition of matrices and multiplication by a number is isomorphic with $\mathcal{H}$. With these definitions, the operator $\hat{A}$ can be identified with the square matrix whose elements are the m^2 numbers $\hat{A}_{ij} = \langle b_i | \hat{A} | b_j \rangle$

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{23m} \\ \dots & \dots & \dots & \dots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \tag{2.170}$$

With these identifications, the components η_i can be rewritten as

$$\eta_i = \sum_j A_{ij} b_j \tag{2.171}$$

This is an expression which is identical to the matrix equation

$$\begin{pmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_m \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{23m} \\ \dots & \dots & \dots & \dots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \dots \\ \gamma_m \end{pmatrix} \tag{2.172}$$

or more succinctly $(\eta_i) = (A_{ij})(b_j)$.

When the above identifications are made we speak of the *matrix representation of $\mathcal{H}$ with respect to the basis* $\{b_i\}$, or simply the $\{b_i\}$-representation of $\mathcal{H}$.

If in a given representation $\hat{A} \Rightarrow (A_{ij})$ and $\hat{A}^\dagger \Rightarrow (A^\dagger_{ij})$, then $A^\dagger_{ij} = A^*_{ji}$; thus, if $\hat{A}$ is hermitian, $A_{ij} = A^*_{ji}$. The representation of the identity operator with respect to any orthonormal basis is the identity matrix (δ_{ij}).

The inverse $\hat{A}^{-1}$ exists if and only if the determinant $det(A_{ij}) \neq 0$; then $A^{-1}_{ij} = cof(A_{ij})/det(A_{ij})$ (cofactors). The matrix elements of a unitary operator $\hat{U}$ satisfy the relation .

Change of Representation - Let $\{|b_i\rangle\}, \{|\bar{b}_i\rangle\}$ be two bases on $\mathcal{H}$. What is the relationship between the representations of a vector $|g\rangle$ and an operator $\hat{A}$ with respect to the bases $\{|b_i\rangle\}$ and $\{|\bar{b}_i\rangle\}$?

Consider first the vector $|g\rangle$ and let $\gamma_i = \langle b_i \,|\, g\rangle$ and $\bar{\gamma}_i = \langle \bar{b}_i \,|\, g\rangle$ be its components along $|b_i\rangle$ and $|\bar{b}_i\rangle$ respectively. Since

$$|\bar{b}_i\rangle = \sum_j \langle b_j \,|\, \bar{b}_i\rangle \, |b_j\rangle \tag{2.173}$$

we have

$$\bar{\gamma}_i = \langle \bar{b}_i \,|\, g\rangle = \sum_j \langle b_j \,|\, \bar{b}_i\rangle \, \langle b_j \,|\, g\rangle \tag{2.174}$$

Defining the matrix $S \Rightarrow (S_{ij}) = \left\langle b_j \,\middle|\, \bar{b}_i \right\rangle$ we can write $\bar{\gamma}_i = (S_{ij})(\gamma_j)$.

The matrix S is unitary in the sense that

$$\sum_k S_{ik} S^*_{jk} = \delta_{ij} \tag{2.175}$$

Instead of thinking of S as a matrix performing a change of bases we can think of it as a unitary operator that generates a *unitary transformation* of *mathcalH* onto itself given by the correspondence

$$\left|\bar{f}\right\rangle = S\left|f\right\rangle \qquad \hat{\bar{A}} = \hat{S}\hat{A}\hat{S}^\dagger \tag{2.176}$$

For any vectors $\left|f\right\rangle, \left|g\right\rangle$ and any operator $\hat{A}$ we then have

$$\left\langle \bar{f} \,\middle|\, \bar{g} \right\rangle = \left\langle f \,|\, g \right\rangle \qquad \left\langle \bar{f} \right| \hat{\bar{A}} \left|\bar{g}\right\rangle = \left\langle f \right| \hat{A} \left|g\right\rangle \tag{2.177}$$

2.14.6 **Projection Operators**

Suppose we have a vector $|\alpha\rangle$ in a separable Hilbert space. The associated projection operator $\hat{P}_\alpha$ is a linear operator in Hilbert space whose action on any other arbitrary vector in the space is to project out the component of that arbitrary vector along the vector $|\alpha\rangle$, i.e.,

$$\hat{P}_\alpha |\beta\rangle = a |\alpha\rangle \tag{2.178}$$

where a is a scalar and $|\beta\rangle$ is any arbitrary vector. This is a projection operator of the entire Hilbert space onto a *one-dimensional subspace*, namely, the single vector $|\alpha\rangle$.

Since, by definition, $\hat{P}_\alpha |\alpha\rangle = |\alpha\rangle$, all projection operators satisfy the following property:

$$\hat{P}_\alpha \hat{P}_\alpha |\beta\rangle = a\hat{P}_\alpha |\alpha\rangle = a |\alpha\rangle = \hat{P}_\alpha |\beta\rangle \tag{2.179}$$

$$(\hat{P}_\alpha^2 - \hat{P}_\alpha)\,|\beta\rangle = 0 \qquad or \qquad \hat{P}_\alpha^2 = \hat{P}_\alpha \tag{2.180}$$

If $|r\rangle$ is an eigenvector of $\hat{P}_\alpha$, such that $\hat{P}_\alpha\,|r\rangle = r\,|r\rangle$, then we have

$$\hat{P}_\alpha^2\,|r\rangle = r\hat{P}_\alpha\,|r\rangle = r^2\,|r\rangle \tag{2.181}$$

$$(\hat{P}_\alpha^2 - \hat{P}_\alpha)\,|r\rangle = (r^2 - r)\,|r\rangle = 0 \tag{2.182}$$

$$r^2 - r = 0 \quad \rightarrow r = 0, 1 \tag{2.183}$$

The *eigenvalues* of any projection operator are $0, 1$.

In general, any operator that satisfies the relation $\hat{A}^2 = \hat{A}$ is called *idempotent* and has eigenvalues 0,1.

Two projection operators $\hat{P}_{\alpha_1}$ and $\hat{P}_{\alpha_2}$ are orthogonal if, for any arbitrary vector $|\beta\rangle$

$$|\eta\rangle = \hat{P}_{\alpha_1}\,|\beta\rangle \text{ and } |\sigma\rangle = \hat{P}_{\alpha_2}\,|\beta\rangle \rightarrow \langle\eta\,|\,\sigma\rangle = 0 \tag{2.184}$$

The scalar constant in the equation $\hat{P}_\alpha \left|\beta\right\rangle = a \left|\alpha\right\rangle$, since it is the component of the arbitrary vector along $\left|\alpha\right\rangle$, is related to the inner product of the arbitrary vector with $\left|\alpha\right\rangle$ by $a = \left\langle\alpha \,|\, \beta\right\rangle$, which implies that

$$\hat{P}_\alpha \left|\beta\right\rangle = \left\langle\alpha \,|\, \beta\right\rangle \left|\alpha\right\rangle = \left(\left|\alpha\right\rangle \left\langle\alpha\right|\right) \left|\beta\right\rangle \tag{2.185}$$

or

$$\hat{P}_\alpha = \left|\alpha\right\rangle \left\langle\alpha\right| \tag{2.186}$$

For an orthonormal basis set $\{\left|q_i\right\rangle\}$, where $\left\langle q_i \,|\, q_j\right\rangle = \delta_{ij}$, we can define a set of projection operators $\{\hat{P}_i\}$, where each projection operator is given by

$$\hat{P}_k = \left|q_k\right\rangle \left\langle q_k\right| \tag{2.187}$$

We then have

$$\hat{P}_i \hat{P}_j = \delta_{ij} \hat{P}_j \quad \text{or} \quad \left|q_i\right\rangle \left\langle q_i\right\rangle \left|q_j\right\rangle \left\langle q_j\right| = \delta_{ij} \left|q_j\right\rangle \left\langle q_j\right| \tag{2.188}$$

so the projection operators are *mutually orthogonal* in this case.

As we stated earlier, the set of projection operators satisfies a *completeness* property, i.e., for any vector we can write

$$|\psi\rangle = \sum_k \langle q_k \,|\, \psi\rangle \, |q_k\rangle = \sum_k |q_k\rangle \, \langle q_k \,|\, \psi\rangle = \sum_k \hat{P}_k \, |\psi\rangle = \left(\sum_k \hat{P}_k \right) |\psi\rangle \tag{2.189}$$

This implies

$$\sum_k \hat{P}_k = \hat{I} = \sum_k |q_k\rangle \, \langle q_k| \tag{2.190}$$

This relation is very powerful and allows us to easily do algebra using the Dirac language by judicious insertion of $\hat{I}$ operators.

Some examples are:

1.

$$\langle \alpha \,|\, \beta\rangle = \langle \alpha| \, \hat{I} \, |\beta\rangle = \sum_k \langle \alpha| \, (|q_k\rangle \, \langle q_k|) \, |\beta\rangle = \sum_k \langle \alpha \,|\, q_k\rangle \, \langle q_k \,|\, \beta\rangle$$

2.

$$\langle\alpha|\,\hat{Q}\,|\beta\rangle = \langle\alpha|\,\hat{I}\hat{Q}\hat{I}\,|\beta\rangle = \langle\alpha|\left(\sum_k |q_k\rangle\,\langle q_k|\right)\hat{Q}\left(\sum_j |q_j\rangle\,\langle q_j|\right)|\beta\rangle$$

$$= \sum_k \sum_j \langle\alpha\,|\,q_k\rangle\,\langle q_k|\,\hat{Q}\,|q_j\rangle\,\langle q_j\,|\,\beta\rangle$$

3.

$$\hat{Q}\,|\beta\rangle = \hat{I}\hat{Q}\,|\beta\rangle = \left(\sum_k |q_k\rangle\,\langle q_k|\right)\hat{Q}\,|\beta\rangle = \sum_k \langle q_k|\,\hat{Q}\,|\beta\rangle\,|q_k\rangle$$

4.

$$\langle\alpha|\,\hat{Q}\hat{R}\,|\beta\rangle = \langle\alpha|\,\hat{I}\hat{Q}\hat{I}\hat{R}\hat{I}\,|\beta\rangle$$

$$= \langle\alpha|\left(\sum_k |q_k\rangle\,\langle q_k|\right)\hat{Q}\left(\sum_k |q_i\rangle\,\langle q_i|\right)\hat{R}\left(\sum_j |q_j\rangle\,\langle q_j|\right)|\beta\rangle$$

$$= \sum_k \sum_j \sum_i \langle\alpha\,|\,q_k\rangle\,\langle q_k|\,\hat{Q}\,|q_i\rangle\,\langle q_i|\,\hat{R}\,|q_j\rangle\,\langle q_j\,|\,\beta\rangle$$

2.14.7 **Unbounded Operators**

Many of the operators we shall deal with in quantum mechanics are not bounded.

An example is easily constructed in the space $L^2(-\infty, \infty)$ of square-integrable functions $f(x)$ for $-\infty < x < \infty$. Let $\hat{X}$ be a linear operator defined by the equation

$$\hat{X} f(x) = x f(x) \tag{2.191}$$

where x is real. This is a Hermitian operator since

$$\begin{aligned}(g, \hat{X} f) &= \int_{-\infty}^{\infty} g^*(x) \hat{X} f(x))\, dx = \int_{-\infty}^{\infty} g^*(x) x f(x)\, dx = \int_{-\infty}^{\infty} x g^*(x) f(x \\ &= \int_{-\infty}^{\infty} [x g(x)]^* f(x))\, dx = \int_{-\infty}^{\infty} [\hat{X} g(x)]^* f(x))\, dx = (\hat{X} g, f)\end{aligned} \tag{2.192}$$

provided that all the integrals converge. It is not bounded since

$$\|\hat{X}f\|^2 = \int_{-\infty}^{\infty} |xf(x)|^2)\,dx \tag{2.193}$$

is not necessarily finite even if

$$\|f\|^2 = \int_{-\infty}^{\infty} |f(x)|^2)\,dx < \infty \tag{2.194}$$

2.15 **Eigenvalues and Eigenvectors of Unitary Operators**

We need to cover a few more details in this area. If $\hat{U}$ is a linear operator which has an inverse $\hat{U}^{-1}$, then the operators $\hat{U}\hat{Q}\hat{U}^{-1}$ and $\hat{Q}$ have the same eigenvalues, that is, if $\hat{Q}\,|\alpha\rangle = \alpha\,|\alpha\rangle$, then

$$\hat{U}\hat{Q}\hat{U}^{-1}(\hat{U}\,|\alpha\rangle) = \hat{U}\hat{Q}\,|\alpha\rangle = \alpha\hat{U}\,|\alpha\rangle \tag{2.195}$$

which says that $\hat{U}\hat{Q}\hat{U}^{-1}$ has the same eigenvalues as $\hat{Q}$ and its eigenvectors are $\hat{U}\,|\alpha\rangle$.

The eigenvectors and eigenvalues of unitary operators have these properties:

1. the eigenvalues are complex numbers of absolute value one
2. two eigenvectors are orthogonal if they correspond to different eigenvalues
3. in a complex finite-dimensional space, the eigenvectors span the space

2.16 **Eigenvalue Decomposition**

Let us now look deeper into the representation of operators in terms of their eigenvalues and eigenvectors.

As we stated earlier, for a finite-dimensional vector space, the eigenvectors of a Hermitian operator always form an orthonormal basis set or they always span the space.

Suppose we have a Hermitian operator $\hat{B}$ with eigenvectors $\{|b_k\rangle, k = 1, 2, 3, \ldots, n\}$ and eigenvalues b_k where

$$\hat{B}\{|b_k\rangle = b_k\{|b_k\rangle \tag{2.196}$$

Labeling the states by the eigenvalues as above will become a standard practice as we get into quantum mechanics.

We showed earlier that we could represent an operator by the expression

$$\hat{B} = \sum_j b_j \left|b_j\right\rangle \left\langle b_j\right| \tag{2.197}$$

in terms of its eigenvalues and the projection operators constructed from the basis set (its eigenvectors).

2.17 **Extension to Infinite-Dimensional Spaces**

We now extend the properties we have been discussing to infinite-dimensional spaces.

First, we extend the properties of projection operators. The projection operators we have been considering are a special case of a more general definition.

In particular, the projection operator we have been discussing $\hat{P}_\alpha = |\alpha\rangle \langle\alpha|$ projects the vector space onto the 1-dimensional subspace spanned by the vector $|\alpha\rangle$.

We extend the definition by defining a projection operator onto larger subspaces.

Let $\hat{E}_M$ be a projection operator onto the subspace M (not necessarily 1-dimensional). This means that for any vector $|\eta\rangle$ in the space, there are unique vectors $|\eta\rangle_{M_\perp}$ in $M^\perp$ which is called the orthogonal complement of M, such that we can always write

$$|\eta\rangle = |\eta\rangle_M + |\eta\rangle_{M_\perp} \tag{2.198}$$

and

$$\hat{E}_M |\eta\rangle = |\eta\rangle_M \tag{2.199}$$

for every $|\eta\rangle$ in the space. The operator $\hat{P}_\alpha = |\alpha\rangle \langle\alpha|$ is clearly a special case where the subspace M contains only one vector, namely, $|\alpha\rangle$.

The more general projection operators $\hat{E}_M$ satisfy all the same properties listed earlier for the single-state projection operators $\hat{P}_\alpha$.

If $\hat{E}_M$ is the projection on the n-dimensional subspace N, one can select an orthonormal basis $\{|b_i\rangle\}$ on $\mathcal{H}$, n of whose vectors $|b_1\rangle, \ldots, |b_n\rangle$ form a basis on N. In the *corresponding representation* $\hat{E}_N$ has the n diagonal matrix elements $(\hat{E}_N)_{kk}$, $k = 1, \ldots, n$ equal to one and all the others equal to zero.

Example: Given the 2-dimensional space C spanned by the basis

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The projection operator onto the 1-dimensional space A ($|b_1\rangle$) is

$$\hat{E}_1 = |b_1\rangle \langle b_1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

The projection operator onto the 1-dimensional space B ($|b_2\rangle$) is

$$\hat{E}_2 = |b_2\rangle \langle b_2| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Note that $A \oplus B = C$, $B = A_\perp$, $A = B_\perp$.

Before proceeding further let us look at the properties of projections and expand on our earlier discussions.

Let $M \subset \mathcal{H}$ be a subspace and $M^\perp$ its orthogonal complement. Every vector $|h\rangle$ can be written in a unique manner as $|h\rangle = |f\rangle + |g\rangle$, with $|f\rangle \in M, |g\rangle \in M^\perp$. $|f\rangle$ is called the orthogonal projection of $|h\rangle$ on M. The linear operator $\hat{E}_M$ defined by $|f\rangle = \hat{E}_M |h\rangle$ is called the projection operator on M. Its domain is the whole space and its range is the subspace M. We say that $\hat{E}_M$ projects on M.

In general, an operator which projects on some subspace is called a projection operator. An operator $\hat{E}$ is a projection operator if and only if $\hat{E}^2 = \hat{E}$ and $\hat{E}^\dagger = \hat{E}$. Let $\hat{E}_M$ and $\hat{E}_N$ be the projections on the subspaces M and N respectively. The product $\hat{E}_M \hat{E}_N$ is a projection if and only if both operators commute, in which case $\hat{E}_M \hat{E}_N$ projects on the intersection of M and N. The sum $\hat{E}_M + \hat{E}_N$ is a projection if and only if $\hat{E}_M \hat{E}_N = 0$, which means that M and N are orthogonal. In that case, $\hat{E}_M + \hat{E}_N$ projects on $M \oplus N$. The difference $\hat{E}_M - \hat{E}_N$ is a projection operator if and only if $\hat{E}_M \hat{E}_N = \hat{E}_N$, which is equivalent to $M \subseteq N$, i.e., N is a subset of M or N is contained in M. In this case $\| \hat{E}_N |f\rangle \| \leq \| \hat{E}_M |f\rangle \|$ for all $|f\rangle \in \mathcal{H}$ and we write $\hat{E}_N \leq \hat{E}_M$.

The dimension of a projection operator $\hat{E}_M$ is the dimension of the range M.

Any two vectors $|f\rangle, |g\rangle$ determine the operator $|f\rangle \langle g|$ defined by

$(|f\rangle\langle g|)\,|h\rangle = \langle g\,|\,h\rangle\,|f\rangle$. We have $(|f\rangle\langle g|)^\dagger = |g\rangle\langle f|$. In particular, $|f\rangle\langle f|$ is Hermitian and, if $|f\rangle$ is normalized, it is the one-dimensional projection whose range is $|f\rangle$.

A subspace M is *invariant* under an operator $\hat{A}$ if for all vectors $|f\rangle \in M$ we have $\hat{A}\,|f\rangle \in M$. If, furthermore, $\hat{A}\,|g\rangle \in M^\perp$ for all $|g\rangle \in M^\perp$, that is, if both M and $M^\perp$ are invariant under $\hat{A}$, then the subspace M is said to reduce the operator $\hat{A}$. The statements "M reduces $\hat{A}$" and "$\hat{A}$ commutes with $\hat{E}_M$" are equivalent.

Let M be invariant under $\hat{A}$. With $|f\rangle$ and $|g\rangle$ given as above, we have

$$(\hat{A}^\dagger\,|g\rangle)^\dagger\,|f\rangle) = (\langle g|\,\hat{A})\,|f\rangle) = \langle g|\,(\hat{A}\,|f\rangle) = \langle g|\,\hat{A}\,|f\rangle = 0 \quad (2.200)$$

Therefore, $\hat{A}^\dagger\,|g\rangle \in M^\perp$ or, equivalently, $M^\perp$ is invariant under $\hat{A}^\dagger$.

From this result, one sees immediately that if M is invariant under the hermitian operator $\hat{B}$, then M reduces $\hat{B}$. The same is true if $\hat{U}$ is unitary because then, from

$$(\hat{U}\,|f\rangle)^\dagger(\hat{U}\,|g\rangle) = \langle f|\,\hat{U}^\dagger\hat{U}\,|g\rangle = \langle f\,|\,g\rangle = 0 \tag{2.201}$$

we conclude that $\hat{U}\,|g\rangle$, being orthogonal to $\hat{U}\,|f\rangle$, must be in $M^\perp$. If no subspaces other than $\mathcal{H}$ (the entire space itself) and $\{0\} = \varnothing$ reduce every member of a set of operators, then the set is called *irreducible*. It follows that a set of operators is irreducible if and only if the only operators that commute with every member of the set are multiples of the identity. If there is a subspace that reduces every operator of the set, then the set is said to be *reducible*. Now let $\hat{W}$ be a hermitian operator with r distinct eigenvalues $\lambda_i, i = 1, \ldots, r$. In addition, let M_i and $\hat{E}_i$ be the eigensubspace and eigenprojection belonging to the eigenvalue λ_i. M_i is invariant under $\mathcal{H}$ and reduces $\hat{W}$ or, equivalently, $\hat{E}_i\hat{W} = \hat{W}\hat{E}_i$. The subspace $M = \oplus_i M_i$ spanned by all the eigenvectors of $\hat{W}$ also reduces $\hat{W}$ and the corresponding projection operator

$$\hat{E} = \sum_i \hat{E}_i \tag{2.202}$$

commutes with $\hat{W}$.

This result has the following important consequence: the *eigenvectors of a Hermitian operator span the whole space*, that is, $\hat{E} = \hat{I}$ or $M =$ entire vector space, which generalizes the ideas we found earlier.

Regarded as an operator on M_i , the operator $\hat{W}$ multiplies every vector by the number λ_i. Therefore, it is equal to $\lambda_i \hat{I}$ and the multiplicity λ_i equals its degeneracy. One can write $\hat{W}$ as the direct sum $\oplus_i \lambda_i \hat{I}_i$ or equivalently, as the sum

$$\sum_i \lambda_i \hat{E}_i \tag{2.203}$$

in terms of the eigenprojections on the vector space.

Collecting together all these results, we have the simplest form of the *spectral theorem* in a unitary space.

To every Hermitian operator $\hat{W}$ on an m-dimensional unitary space there corresponds a unique family of non-zero projection operators, the eigenprojections of the space,
$\hat{E}_i$, $i = 1, \ldots, r$, $r \leq m$ with the following properties:

1. The projections $\hat{E}_i$ are pairwise orthogonal

$$\hat{E}_i \hat{E}_j = \hat{E}_i \delta_{ij} \tag{2.204}$$

2. The family of projections is complete

$$\sum_i \hat{E}_i = \hat{I} \tag{2.205}$$

3. There exists a unique set of r distinct real numbers λ_i, the eigenvalues of $\hat{W}$, such that

$$\hat{W} = \sum_{i=1}^{r} \lambda_i \hat{E}_i \tag{2.206}$$

This expression is the *spectral resolution* of $\hat{W}$.

The range of $\hat{E}_i$ is the eigensubspace M_i belonging to λ_i. Its dimension is the degeneracy or multiplicity s_i of λ_i. On it one can construct an orthonormal basis $\{|b_i^r\rangle\,,\ r = 1, \ldots, s_i$. It follows from the completeness of the family $\hat{E}_i$ that the union of all those bases $\{|b_i^r\rangle\,,\ r = 1, \ldots, s_i,\ i = 1, \ldots, m$ constitutes an orthonormal basis on the vector space One often expresses this fact by saying that $\hat{W}$ possesses a *complete set* of eigenvectors.

It is an immediate consequence of (1) and (2) above that for every vector $|f\rangle$ we have $\langle f|\,\hat{E}_i\,|f\rangle \geq 0$ and

$$\sum_i \langle f|\,\hat{E}_i\,|f\rangle = 1 \tag{2.207}$$

that is, for each vector and each family of projections, the set of numbers $P_i = \langle f|\,\hat{E}_i\,|f\rangle$ constitutes a so-called *discrete probability distribution.* This will be of fundamental importance in quantum theory as we shall see later.

Two hermitian operators

$$\sum_i \alpha_i \hat{E}_i \quad and \quad \sum_i \beta_i \hat{F}_i \tag{2.208}$$

commute if and only if every pair $\hat{E}_i, \hat{F}_i$ of their eigenprojections commute.

From the orthogonality of the projections in the spectral resolution of $\hat{W}$ we have for every normalized vector $|f\rangle$

$$\|\hat{W}\,|f\rangle\,\|^2 = \langle f|\,\hat{W}^2\,|f\rangle = \sum_i \lambda_i^2\,\langle f|\,\hat{E}_i\,|f\rangle \leq \lambda_m^2 \tag{2.209}$$

where λ_m is the largest eigenvalue and the equality holds for $|f\rangle$ in the range of $\hat{E}_m$. It follows that the norm of $\hat{W}$ is $|\lambda_m|$.

Functions of a Hermitian Operator - Using the spectral resolution of a Hermitian operator

$$\hat{Q} = \sum_{i=1}^{r} \lambda_i \hat{E}_i \tag{2.210}$$

one can verify that for a non-negative integer n one has

$$\hat{Q}^n = \sum_{i=1}^{r} \lambda_i^n \hat{E}_i \tag{2.211}$$

(also valid for negative n if all λ_i are non-zero).

This property suggests the following *definition* of a function of a Hermitian operator.

If $F(x)$ is a complex-valued function of the real variable x, then the function $F(\hat{Q})$ of the Hermitian operator $\hat{Q}$ is the operator

$$F(\hat{Q}) = \sum_i F(\lambda_i)\hat{E}_i \tag{2.212}$$

Now, as we saw above, for every vector $|f\rangle$ the family of projections $\hat{E}_i$ belonging to a Hermitian operator determines a probability distribution on a discrete finite sample space with the probabilities given by $P_i = \langle f| \hat{E}_i |f\rangle$.

In probability theory, the passage to a discrete but infinite sample space offers no difficulty; the sums that yield averages are simply replaced by convergent series. The difficulties appear in the case where the sample space is continuous. One cannot then construct the probabilities for every possible set of outcomes from the probabilities of the points of the space (it is in general zero). Instead, one must consider the probabilities of appropriate elementary sets which, in the one-dimensional sample space in which we are interested here, can be taken to be intervals of the real line.

To discuss such a case it is convenient to introduce the probability distribution function $D(\alpha)$ defined as the probability that the outcome of a trial is (less than) α.

In the discrete case, let P_i be the probability that the outcome of a trial yields the value ξ_i and let us order the indices in such a way $\xi_i < \xi_j$ for $i < j$. Written in terms of the P_i the distribution function is

$$D(\alpha) = \sum_{i=-\infty}^{i_\alpha} P_i \tag{2.213}$$

where i_α is the largest index such that $\xi_i < \alpha$ (we are assuming that the sample space is infinite, but the finite case is included if we put the appropriate $P_i = 0$). The function $D(\alpha)$ is clearly a non-decreasing *ladder function* with the properties $D(-\infty) = 0$, $D(\infty) = 1$. We have chosen the upper limit in the summation so as to satisfy the *convention* that $D(\alpha)$ is continuous on the right.

One can imagine a pure continuous sample space as the limit of a discrete one when the differences $\xi_{i+1} - \xi_i$ tend to zero. The distribution function then becomes the limit of a ladder function with the properties just mentioned. It is, therefore, a continuous non-decreasing function $D(\alpha)$ such that
$D(-\infty) = 0$, $D(\infty) = 1$. In the case where $D(\alpha)$ is everywhere differentiable, as is the case in most physical problems, the probability density $\pi(\alpha)$ is defined by $D'(\alpha) = dD(\alpha)/d\alpha$ and the average of the random variable $f(\alpha)$ is given by

$$\langle f(\alpha) \rangle = \int f(\alpha)\pi(\alpha)\, d\alpha \tag{2.214}$$

In the general case, the sample space is continuous but includes non-zero probability P_i concentrated at a countable number of points α_i. In this case $D(\alpha)$ will have a countable number of discontinuities of size P_i. If $D(\alpha)$ is differentiable everywhere else and $\pi(\alpha)$ is the corresponding probability density, then we have

$$\langle f(\alpha) \rangle = \int_{-\infty}^{\infty} f(\alpha)\pi(\alpha)\, d\alpha + \sum_i f(\alpha_i) P_i \tag{2.215}$$

Alternatively, using the Dirac δ-function we can write

$$\langle f(\alpha)\rangle = \int_{-\infty}^{\infty} f(\alpha)\pi_d(\alpha)\, d\alpha \tag{2.216}$$

where $\pi_d(\alpha)$ is the derivative of $D(\alpha)$, that is,

$$\pi_d(\alpha) = \pi(\alpha) + \sum_i P_i \delta(\alpha - \alpha_i) \tag{2.217}$$

The average can also be conveniently written by using the *Stieltjes integral* defined for a function $g(\alpha)$ with a countable number of discontinuities by

$$\int_a^b f(\alpha)\, dg(\alpha) = lim \sum_{i=1}^{n} f(\alpha_i)[g(\alpha_i) - g(\alpha_{i-1})] \tag{2.218}$$

where the α_i,$(a = \alpha_0 \leq \alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_n = b)$ form a subdivision of the interval (a, b) and the limit is taken over a sequence of ever finer subdivisions.

In terms of the Stieltjes integral we then have

$$\langle f(\alpha)\rangle = \int_{-\infty}^{\infty} f(\alpha)\, dD(\alpha) \tag{2.219}$$

Now let us consider a Hermitian operator $\hat{B}$ in an infinite-dimensional space. We label its discrete eigenvalues in order of increasing eigenvalue where we assume

$$b_1 < b_2 < b_3 < \ldots < b_{m-1} < b_m \quad and \quad \hat{B}\,|b_j\rangle = b_j\,|b_j\rangle \tag{2.220}$$

For each real number x we define the operator

$$\hat{E}_x = \sum_{b_j<x} \hat{P}_j = \sum_{b_j<x} |b_j\rangle\,\langle b_j| \tag{2.221}$$

With this definition, $\hat{E}_x$ is the projection operator onto the subspace spanned by all eigenvectors with eigenvalues $b_k < x$. If $x < b_1$ (the smallest eigenvalue), then

$\hat{E}_x$ is zero (no terms in the sum) and if $x > b_m$ (the largest eigenvalue), then $\hat{E}_x = \hat{I}$ because of the completeness property

$$\sum_{k=1}^{m} \hat{P}_k = \hat{I} \tag{2.222}$$

$\hat{E}_x$ increases from zero to one as x increases through the *spectrum* of eigenvalues. In fact, $\hat{E}_x$ increases(jumps) by an amount $\hat{P}_k$ when x reaches the eigenvalue b_k.

For each x let us define $d\hat{E}_x = \hat{E}_x - \hat{E}_{x-\epsilon}$ where ϵ is positive and small enough so that there is no eigenvalue b_j such that $(x - \epsilon) \leq b_j < x$. This means that $d\hat{E}_x$ is not zero only when x is an eigenvalue b_k and $d\hat{E}_x = \hat{P}_k$ for $x = b_k$.

Let us say this very important stuff in still another way.

In a unitary space, the family of projections $\hat{E}_i$ belonging to a hermitian operator

$$\hat{A} = \sum_i \xi_i \hat{E}_i \tag{2.223}$$

can be thought of as constituting a probability distribution on a finite sample space of operators. We shall take the eigenvalues to be ordered in ascending order. For every vector $|f\rangle$ the *operator valued probability* $\hat{E}_i$ generates the ordinary probability distribution $P_i = \langle f| \hat{E}_i |f\rangle$, which in quantum mechanics will give the probability of the outcome ξ_i upon measurement of $\hat{A}$ on a system in the state $|f\rangle$ as we shall see.

In analogy with ordinary probability ideas one can construct a corresponding *operator valued probability distribution function*

$$\hat{E}(\alpha) = \sum_{-\infty}^{i_\alpha} \hat{E}_i \tag{2.224}$$

A formula that one would expect to also be applicable in the case of the infinite-dimensional Hilbert space if the operator $\hat{A}$ corresponds to an observable which yields upon measurement a countable set of possible values.

From the properties of the family $\hat{E}_i$ it follows that $\hat{E}(\alpha)$ is a projection operator, that $\hat{E}(\alpha)$ and $\hat{E}(\alpha')$ commute, that we have $\hat{E}(\alpha') \geq \hat{E}(\alpha)$ for $\alpha' > \alpha$ and that $\hat{E}(-\infty) = 0, \hat{E}(\infty) = \hat{I}$. $\hat{E}(\alpha)$ is an operator valued *ladder* function whose jumps at the discontinuities are given by $\hat{E}(\xi_i) - \hat{E}(\xi_i -) = \hat{E}_i$.

Quantum mechanics will require that we consider operators on the Hilbert space that will correspond to observables that yield upon measurement a continuous range of possible values. Such operators are associated with *operator valued probability distribution functions* analogous to the continuous distribution functions of ordinary probability, that is, with a family of projections $\hat{E}(\alpha)$ depending continuously on the parameter α such that $\hat{E}(\alpha') \geq \hat{E}(\alpha)$ for $\alpha' > \alpha$ and that $\hat{E}(-\infty) = 0, \hat{E}(\infty) = \hat{I}$. In the most general case corresponding to the continuous sample space with points ξ_i of concentrated probability we would expect the family $\hat{E}(\alpha)$ to have discontinuities at ξ_i of the form $\hat{E}(\xi_i) - \hat{E}(\xi_i -) = \hat{E}_i$ where $\hat{E}_i$ is the *operator valued probability* concentrated at the point ξ_i.

A *spectral family* is a one parameter family of commuting projection operators $\hat{E}(\alpha)$ depending on the real parameter α that satisfies the following properties:

1. $\hat{E}(\alpha)$ is increasing: $\hat{E}(\alpha') \geq \hat{E}(\alpha)$ for $\alpha' > \alpha$
2. $\hat{E}(\alpha)$ is continuous on the right: $\hat{E}(\alpha') \to \hat{E}(\alpha)$ for $\alpha' \to \alpha$ and $\alpha' > \alpha$
3. $\hat{E}(\alpha)$ is complete: $\hat{E}(-\infty) = 0, \hat{E}(\infty) = \hat{I}$

It follows that $\hat{E}(\alpha)\hat{E}(\alpha') = \hat{E}(\alpha')\hat{E}(\alpha) = \hat{E}(\alpha)$ for $\alpha' > \alpha$.

The tentative conclusions of this intuitive discussion can, in fact, be proven to be correct. We now formulate them precisely.

In place of

$$\sum_{k=1}^{m} = \hat{I} \tag{2.225}$$

we can now *formally* write

$$\int_{-\infty}^{\infty} d\hat{E}_x = \hat{I} \tag{2.226}$$

and in place of

$$\hat{B} = \sum_{j=1}^{m} b_j \left|b_j\right\rangle \left\langle b_j\right| \tag{2.227}$$

we can now *formally* write

$$\hat{B} = \int_{-\infty}^{\infty} x \, d\hat{E}_x \tag{2.228}$$

Additionally, we have

$$\left\langle \alpha \,|\, \beta \right\rangle = \int_{-\infty}^{\infty} d \left\langle \alpha \right| \hat{E}_x \left|\beta\right\rangle \qquad \left\langle \alpha \right| \hat{B} \left|\beta\right\rangle = \int_{-\infty}^{\infty} x \, d \left\langle \alpha \right| \hat{E}_x \left|\beta\right\rangle \tag{2.229}$$

We can easily show the validity of these expressions in the case of a finite-dimensional space with discrete eigenvalues. In this case, we can satisfy all of the properties of $\hat{E}_x$ by writing

$$\hat{E}_x = \sum_k \hat{P}_k \theta(x - b_k) \tag{2.230}$$

where

$$\theta(x - b_k) = \begin{cases} +1 & \text{if} \quad x > b_k \\ 0 & \text{if} \quad x < b_k \end{cases} \tag{2.231}$$

This is called the *Heaviside step function.*

Then

$$d\hat{E}_x = \sum_k \hat{P}_k \, d\theta(x - b_k) = \sum_k \hat{P}_k \, \frac{d}{dx}\theta(x - b_k) \, dx = \sum_k \hat{P}_k \delta(x - b_k) \, dx \tag{2.232}$$

where

$$\delta(x-c) = Dirac\ \delta - function = 0 \quad if \quad x \neq c \tag{2.233}$$

and satisfies

$$\int_{-\infty}^{\infty} \delta(x-c)\, dx = 1 \tag{2.234}$$

In addition, we have used

$$\int_{-\infty}^{\infty} g(x)\delta(x-c)\, dx = g(c) \tag{2.235}$$

In the finite-dimensional case, we then have

$$\int_{-\infty}^{\infty} d\hat{E}_x = \int_{-\infty}^{\infty} \sum_k \hat{P}_k \delta(x-b_k)\, dx = \sum_k \hat{P}_k = \hat{I} \tag{2.236}$$

$$\int_{-\infty}^{\infty} x\, d\hat{E}_x = \int_{-\infty}^{\infty} x \sum_k \hat{P}_k \delta(x-b_k)\, dx = \sum_k b_k \hat{P}_k = \hat{B} \tag{2.237}$$

$$\int_{-\infty}^{\infty} d\,\langle\alpha|\,\hat{E}_x\,|\beta\rangle = \int_{-\infty}^{\infty} \sum_k \langle\alpha|\,\hat{P}_k\,|\beta\rangle\,\delta(x-b_k)\,dx$$

$$= \sum_k \langle\alpha|\,\hat{P}_k\,|\beta\rangle = \langle\alpha|\left(\sum_k \hat{P}_k\right)|\beta\rangle = \langle\alpha\,|\,\beta\rangle \qquad (2.238)$$

$$\int_{-\infty}^{\infty} x\,d\,\langle\alpha|\,\hat{E}_x\,|\beta\rangle = \int_{-\infty}^{\infty} x \sum_k \langle\alpha|\,\hat{P}_k\,|\beta\rangle\,\delta(x-b_k)\,dx$$

$$= \sum_k b_k\,\langle\alpha|\,\hat{P}_k\,|\beta\rangle = \langle\alpha|\left(\sum_k b_k\hat{P}_k\right)|\beta\rangle = \langle\alpha|\,\hat{B}\,|\beta\rangle \quad (2.239)$$

where we have used the fact that $\langle\alpha|\,\hat{E}_x\,|\beta\rangle$ is a complex function of x which jumps in value by the amount $\langle\alpha|\,\hat{P}_k\,|\beta\rangle$ at $x = b_k$.

So, we see that result

$$\hat{E}_x = \sum_k \hat{P}_k \theta(x - b_k) \tag{2.240}$$

works in the finite-dimensional case!!!

Unitary operators can be handled in the same manner. We label the eigenvalues (absolute value = 1) of the unitary operator $\hat{U}$ by $u_k = e^{i\theta_k}$ with the θ-values labeled in order

$$0 < \theta_1 < \theta_2 < \ldots < \theta_{m-1} < \theta_m, 2\pi \tag{2.241}$$

As before we define

$$\hat{E}_x = \sum_{\theta_j < x} \hat{P}_j = \sum_{\theta_j < x} |u_j\rangle \langle u_j| \tag{2.242}$$

This operator now projects onto the subspace spanned by all eigenvectors for eigenvalues $u_k = e^{i\theta_k}$ with $\theta_k < x$. If $x \leq 0$, then $\hat{E}_x = 0$. If $x \geq 2\pi$, then $\hat{E}_x = \hat{I}$. $\hat{E}_x$ increments by $\hat{P}_k$ (the same as for a Hermitian operator) at the eigenvalues $u_k = e^{i\theta_k}$.

We can then write

$$\hat{U} = \sum_{k=1}^{m} u_k \hat{P}_k = \sum_{k=1}^{m} e^{i\theta_k} \hat{P}_k \rightarrow \int_0^{2\pi} e^{ix} \, d\hat{E}_x \tag{2.243}$$

and

$$\langle \alpha | \, \hat{U} \, | \beta \rangle = \int_0^{2\pi} e^{ix} \, d \, \langle \alpha | \, \hat{E}_x \, | \beta \rangle \tag{2.244}$$

Summarizing, for every Hermitian operator $\hat{H}$ there corresponds a unique spectral family $\hat{E}_H(\alpha)$ that commutes with $\hat{H}$ such that for every $|f\rangle$ and every $|g\rangle$ in the domain of $\hat{H}$

$$\langle f|\,\hat{H}\,|g\rangle = \int_{-\infty}^{\infty} \alpha\, d\,\langle f|\,\hat{E}_H(\alpha)\,|g\rangle \tag{2.245}$$

where the integral is a Riemann-Stieltjes integral. This expression can be written in short as

$$\hat{H} = \int_{-\infty}^{\infty} \alpha\, d\hat{E}_H(\alpha) \tag{2.246}$$

and is called the *spectral resolution* of $\hat{H}$. We have

$$\hat{E}_H(\alpha) = \int_{-\infty}^{\alpha} d\hat{E}_H(\alpha') \tag{2.247}$$

and therefore

$$\hat{I} = \int_{-\infty}^{\infty} d\hat{E}_H(\alpha) \tag{2.248}$$

Now to every interval $\Delta = (\alpha_1, \alpha_2)$ of the real line, there corresponds a projection operator

$$\hat{E}_H[\Delta] = \int_{\alpha_1}^{\alpha_2} d\hat{E}_H(\alpha) = \hat{E}_H(\alpha_2) - \hat{E}_H(\alpha_1) \tag{2.249}$$

This is a definition that can be extended to a set of intervals. It follows from the properties of the spectral family $\hat{E}_H(\alpha)$ that

$$\hat{E}_H[\Delta]\hat{E}_H[\Delta'] = \hat{E}_H[\Delta \cap \Delta'] \tag{2.250}$$

and

$$\hat{E}_H[\Delta] + \hat{E}_H[\Delta'] = \hat{E}_H[\Delta \cup \Delta'] \tag{2.251}$$

The quantity $d\hat{E}_H(\alpha)$ can be thought of as the projection $\hat{E}_H(d\alpha)$ corresponding to an infinitesimal interval of length $d\alpha$ centered at α.

By definition of the Stieltjes integral one has

$$\hat{H} = \lim_{n\to\infty} \sum_{\Delta_j \in S_n} \alpha_j \hat{E}_H[\Delta_j] \tag{2.252}$$

where $\{S_n\}$ is a sequence of subdivisions of the real line, such that S_n becomes infinitely fine as $n \to \infty$. The sum runs over all the intervals $\Delta_j^{(n)} = \alpha_j^{(n)} - \alpha_{j-1}^{(n)}$ of the subdivision S_n. If the spectral family $\hat{E}_K(\alpha)$ belonging to a Hermitian operator $\hat{K}$ is constant except for a countable number of isolated discontinuities at the points α_i of size $\hat{E}_K(\alpha_i) - \hat{E}_K(\alpha_i -) = \hat{E}_i$, then $\hat{K}$ has a spectral resolution entirely similar to the one in unitary space

$$\hat{K} = \sum_i \alpha_i \hat{E}_i \tag{2.253}$$

although in this case the number of terms in the sum may be infinite.

A general operator $\hat{H}$ can be regarded as the limit of a sequence

$$\hat{H}_n = \sum_{\Delta_j \in S_n} \alpha_j \hat{E}_H[\Delta_j] \tag{2.254}$$

of operators of type $\hat{K}$.

Let $\hat{A}$ and $\hat{B}$ be two operators with spectral families $\hat{E}_A(\alpha), \hat{E}_B(\alpha)$. Suppose that $\hat{A}$ and $\hat{B}$ commute in the sense that $[\hat{A}, \hat{B}]\,|g\rangle = 0$ for every $|g\rangle$ in the domain of $[\hat{A}, \hat{B}]$, then one can show that

$$[\hat{E}_A(\alpha), \hat{E}_B(\alpha)]\,|g\rangle = 0 \tag{2.255}$$

However, unless the domain of $[\hat{A}, \hat{B}]$ coincides with the whole space, this relation does not imply that the spectral families commute. For this reason, when we deal with two operators $\hat{A}$ and $\hat{B}$ that possess a spectral family we shall use a stronger definition of commutativity:

$\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ commute if their spectral families commute.

2.18 Spectral Decomposition - More Details

It turns out that for infinite-dimensional vector spaces there exist Hermitian and unitary operators that have no eigenvectors and eigenvalues.

Consider the eigenvalue equation

$$-i\frac{d}{dx}\psi(x) = \hat{D}\psi(x) = \beta\psi(x) \tag{2.256}$$

This is a differential equation whose solution is

$$\psi(x) = ce^{i\beta x} \qquad c = constant \tag{2.257}$$

Suppose the operator

$$\hat{D} = -i\frac{d}{dx} \tag{2.258}$$

is defined on the interval $a \leq x \leq b$. Then its adjoint operator $\hat{D}^\dagger$ is defined by the relation

$$\langle\phi|\,\hat{D}^\dagger\,|\psi\rangle = \langle\psi|\,\hat{D}\,|\phi\rangle^* \tag{2.259}$$

or for function spaces

$$\int_a^b \phi^*(x)\hat{D}^\dagger\psi(x)\,dx = \left\{\int_a^b \psi^*(x)\hat{D}\phi(x)\,dx\right\}^* = \int_a^b \phi^*(x)\hat{D}\psi(x)\,dx + i\left[\psi(x)\phi^*(x)\right]\Big|_a^b \tag{2.260}$$

where the last step follows from an integration by parts. If boundary conditions are imposed so that the last term(called the *surface* term) vanishes, then $\hat{D}$ will be a Hermitian operator; otherwise it is not Hermitian.

Now let us try to find the eigenvectors (eigenfunctions in this case) within a particular vector space. It turns out that we can define several different vector spaces *depending on the boundary conditions* that we impose.

Case 1: No boundary conditions

In this case, all complex β are eigenvalues and $\hat{D}$ is not Hermitian. In quantum mechanics we will be interested in Hermitian operators, so we are not really interested in this case.

Case 2: $a = -\infty$, $b = +\infty$ with $|\psi(x)|$ bounded as $|x| \to \infty$

All real values of β are eigenvalues. The eigenfunctions $\psi(x)$ are not normalizable since

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = |c|^2 \int_{-\infty}^{\infty} dx = \infty \tag{2.261}$$

They do, however, form a complete set in the sense that an arbitrary function can be represented as a the Fourier integral

$$q(x) = \int_{-\infty}^{\infty} F(\beta) e^{i\beta x} \, d\beta \tag{2.262}$$

which may be regarded as a continuous linear combination of the eigenfunctions. In this case, $F(\beta)$ is the *Fourier transform* of $q(x)$.

Case 3: $a = -\frac{L}{2}$, $b = +\frac{L}{2}$ with periodic boundary conditions $\psi(-\frac{L}{2}) = \psi(\frac{L}{2})$

The eigenvalues form a discrete set, β_n, satisfying

$$e^{-i\beta_n \frac{L}{2}} = e^{i\beta_n \frac{L}{2}} \rightarrow e^{i\beta_n L} = 1 \tag{2.263}$$

which implies

$$\beta_n L = 2n\pi \rightarrow \beta_n = \frac{2n\pi}{L} \tag{2.264}$$

where $n =$ integers such that $-\infty \leq n \leq \infty$. These eigenfunctions form a complete orthonormal set (normalize by choosing the constant c appropriately) and $\hat{D}$ is Hermitian. The completeness of the eigenfunction set follows from the theory of Fourier series.

Case 4: $a = -\infty$, $b = +\infty$ with $\psi(x) \to 0$ as $|x| \to \infty$

In this case, the operator $\hat{D}$ is Hermitian (the surface term vanishes), but it has no eigenfunctions within the space.

So, a Hermitian operator on an infinite-dimensional space may or may not possess a complete set of eigenfunctions, depending on the precise nature of the operator and the vector space.

It turns out, however, that the decomposition into projection operators can be reformulated in a way that does not rely on the existence of eigenfunctions. This alternative formulation uses the integral form of the projection operators derived earlier.

We need, however, to remind ourselves of some ideas we stated above(since it never hurts to repeat important stuff).

Let $\hat{E}_1$ and $\hat{E}_2$ be projection operators onto subspaces M_1 and M_2, respectively.

We say that $\hat{E}_1$ and $\hat{E}_2$ are *orthogonal* if M_1 and M_2 are orthogonal (every vector in M_1 is orthogonal to every vector in M_2). We can express this orthogonality, in general, using the relation

$$\hat{E}_j \hat{E}_k = \delta_{jk} \hat{E}_k \tag{2.265}$$

If M_1 is *contained* in M_2, we write $\hat{E}_1 \leq \hat{E}_2$. This means that either $\hat{E}_1 \hat{E}_2 = \hat{E}_1$ or $\hat{E}_2 \hat{E}_1 = \hat{E}_1$. If $\hat{E}_1 \leq \hat{E}_2$, then $\| \hat{E}_1 |\alpha\rangle \| \leq \| \hat{E}_2 |\alpha\rangle \|$ for any vector $|\alpha\rangle$. If $\hat{E}_1 \hat{E}_2 = \hat{E}_2 \hat{E}_1$, then $\hat{E}_1 \hat{E}_2$ is a projection operator that projects onto the subspace which is the *intersection* of M_1 and M_2 , that is, the set of all vectors that are in both M_1 and M_2.

If $\hat{E}_1$ and $\hat{E}_2$ are orthogonal, then $\hat{E}_1 + \hat{E}_2$ is the projection operator onto $M_1 \oplus M_2$ (the direct sum).

If $\hat{E}_1 \leq \hat{E}_2$, $\hat{E}_1 - \hat{E}_2$ is the projection operator onto the subspace which is the orthogonal complement of M_1 in M_2, that is, the set of vectors in M_2 which are orthogonal to every vector in M_1.

Definition: A family of projection operators $\hat{E}_x$ depending on a real parameter x is a *spectral family* if it has the following properties:

1. if $x \leq y$ then $\hat{E}_x \leq \hat{E}_y$ or $\hat{E}_x \hat{E}_y = \hat{E}_x = \hat{E}_y \hat{E}_x$ – this means that $\hat{E}_x$ projects onto the subspace corresponding to eigenvalues $\leq x$.
2. if ϵ is positive, then $\hat{E}_{x+\epsilon} |\eta\rangle \to \hat{E}_x |\eta\rangle$ as $\epsilon \to 0$ for any vector $|\eta\rangle$ and any x.
3. $\hat{E}_x |\eta\rangle \to |0\rangle$ (the null vector) as $x \to -\infty$ and $\hat{E}_x |\eta\rangle \to |\eta\rangle$ as $x \to \infty$ for any vector $|\eta\rangle$.

For each *self-adjoint* operator $\hat{B}$ there is a unique spectral family of projection operators $\hat{E}_x$ such that

$$\langle\gamma|\,\hat{B}\,|\eta\rangle = \int_{-\infty}^{\infty} x\, d\,\langle\gamma|\,\hat{E}_x\,|\eta\rangle \tag{2.266}$$

for all vectors $|\eta\rangle$ and $|\gamma\rangle$. We then write

$$\hat{B} = \int_{-\infty}^{\infty} x\, d\hat{E}_x \tag{2.267}$$

This is called the *spectral decomposition* or *spectral resolution* of $\hat{B}$.

The same results hold for unitary operators. For each unitary operator $\hat{U}$ there is a unique spectral family of projection operators $\hat{E}_x$ such that $\hat{E}_x = 0$ for $x \leq 0$ and $\hat{E}_x = 1$ for $x \geq 2\pi$ and

$$\langle\gamma|\,\hat{U}\,|\eta\rangle = \int_{0}^{2\pi} e^{ix}\, d\,\langle\gamma|\,\hat{E}_x\,|\eta\rangle \tag{2.268}$$

for all vectors $|\eta\rangle$ and $|\gamma\rangle$.

We then write

$$\hat{U} = \int_0^{2\pi} e^{ix}\, d\hat{E}_x \tag{2.269}$$

This is called the *spectral decomposition* or *spectral resolution* of $\hat{U}$.

Both of these results generalize for functions of an operator, i.e.,

$$g(\hat{B}) = \int_{-\infty}^{\infty} g(x)\, d\hat{E}_x \tag{2.270}$$

We considered the case of a discrete spectrum of eigenvalues earlier and found that when the operator $\hat{B}$ has the eigenvalue equation

$$\hat{B}\,|b_k\rangle = b_k\,|b_k\rangle \tag{2.271}$$

we then have

$$\hat{E}_x = \sum_k \hat{P}_k \theta(x - b_k) = \sum_k |b_k\rangle\,\langle b_k|\,\theta(x - b_k) \tag{2.272}$$

so that

$$d\hat{E}_x = \sum_k |b_k\rangle \langle b_k| \, \delta(x - b_k) \, dx \tag{2.273}$$

which implies that the only contributions to the integral occur at the eigenvalues b_k.

We can state all of this stuff *even more formally* once again

The Eigenvalue Problem and the Spectrum

Based on our previous discussion, we can now say that the eigenvalue problem $\hat{H} |f\rangle = \lambda |f\rangle$ has solutions if and only if the spectral family $\hat{E}_H(\alpha)$ is discontinuous. The eigenvalues λ_i are the points of discontinuity of $\hat{E}_H(\alpha)$. The eigenprojection $\hat{E}_i$ belonging to λ_i is the discontinuity of $\hat{E}_H(\alpha)$ at λ_i:

$$\hat{E}_i = \hat{E}_H(\lambda_i) - \hat{E}_H(\lambda_i -) \tag{2.274}$$

It follows that the eigenprojections are orthogonal and that (for hermitian $\hat{H}$) the eigenvalues are real.

The *spectrum* of $\hat{H}$ consists of the set Σ of points of the real axis where the spectral family $\hat{E}_H(\alpha)$ is increasing. If the spectral family is constant except for a (necessarily countable) number of discontinuities $\hat{H}$ is said to have a *pure discrete* spectrum. If the spectral family is everywhere continuous $\hat{H}$ is said to have a *pure continuous* spectrum. Otherwise the spectrum is said to be *mixed*. If and only if $\hat{H}$ is bounded (positive) is its spectrum bounded (positive). Since the points of constancy of $\hat{E}_H(\alpha)$ do not contribute to the integral in

$$\hat{H} = \int_{-\infty}^{\infty} \alpha \, d\hat{E}_H(\alpha) \tag{2.275}$$

the region of integration can be restricted to the spectrum and we can write

$$\hat{H} = \int_{\Sigma} \alpha \, d\hat{E}_H(\alpha) \tag{2.276}$$

Suppose that an operator $\hat{H}$ has a mixed spectrum Σ. The subspace M spanned by its eigenvectors reduces $\hat{H}$ so that we can write $\hat{H} = \hat{H}_d \oplus \hat{H}_c$ where $\hat{H}_d$ and $\hat{H}_c$ are operators on M and $M^\perp$, respectively. The spectrum Σ_d of $\hat{H}_d$ is pure discrete and is called the *discrete spectrum* of $\hat{H}$ while the spectrum Σ_c of $\hat{H}_c$ is pure continuous and is called the *continuous spectrum* of $\hat{H}$. Note that $\Sigma = \Sigma_d \cup \Sigma_c$, but that Σ_d and Σ_c may have points in common, that is, there may be eigenvalues embedded in the continuous spectrum. Separating out the discrete spectrum, the spectral resolution of $\hat{H}$ can be written

$$\hat{H} = \sum_i \alpha_i \hat{E}_i + \int_{\Sigma_c} \alpha \, d\hat{E}_H(\alpha) \quad , \quad \alpha_i \in \Sigma_d \tag{2.277}$$

Clearly, the terms on the RHS are, respectively $\hat{H}_d$ and $\hat{H}_c$, and when regarded as operators on the vector space.

Now let us consider the case of a *continuous spectrum* of eigenvalues. In particular, consider the multiplicative operator $\hat{Q}$ defined on $L^2(-\infty, \infty)$ by

$$\hat{Q}g(x) = xg(x) \tag{2.278}$$

for all functions $g(x)$ in $L^2(-\infty, \infty)$. This is a Hermitian operator since

$$\begin{aligned}\int_a^b \phi^*(x)\hat{Q}^\dagger\psi(x)\,dx &= \left\{\int_a^b \psi^*(x)\hat{Q}\phi(x)\,dx\right\}^* = \left\{\int_a^b \psi^*(x)x\phi(x)\,dx\right\}^* \\ &= \int_a^b \phi^*(x)x\psi(x)\,dx = \int_a^b \phi^*(x)\hat{Q}\psi(x)\,dx\end{aligned} \tag{2.279}$$

Now suppose that $\hat{Q}$ has an eigenvalue equation with eigenfunctions $q(x)$ in $L^2(-\infty, \infty)$ of the form

$$\hat{Q}q(x) = \beta q(x) \tag{2.280}$$

Since all functions in $L^2(-\infty, \infty)$, including $q(x)$, must also satisfy $\hat{Q}g(x) = xg(x)$, we then have

$$\hat{Q}q(x) = xq(x) = \beta q(x) \quad or \quad (x-\beta)q(x) = 0 \qquad for\ all\ x \tag{2.281}$$

The formal solution to this equation is the Dirac δ-function

$$q(x) = \delta(x-\beta) \tag{2.282}$$

The spectral theorem still applies to this operator. The projection operators for $\hat{Q}$, in this case, are given by

$$\hat{E}_\beta g(x) = \theta(\beta - x)g(x) \tag{2.283}$$

This is equal to $g(x)$ if $x < \beta$ and is 0 for $x > \beta$. We then have

$$\hat{Q} = \int_{-\infty}^{\infty} \beta \, d\hat{E}_\beta \tag{2.284}$$

which can be easily verified by

$$\hat{Q}g(x) = \int_{-\infty}^{\infty} \beta \, d\hat{E}_\beta g(x) = \int_{-\infty}^{\infty} \beta \, d[\theta(\beta - x)g(x)]$$
$$= \int_{-\infty}^{\infty} \beta \frac{d}{d\beta}[\theta(\beta - x)g(x)] \, d\beta = \int_{-\infty}^{\infty} \beta\delta(\beta - x)g(x)] \, d\beta = xg(x) \tag{2.285}$$

So the decomposition into projection operators can still be defined in the case of a continuous spectrum.

Saying it still another way. Let $\hat{E}_Q(x)$ be its spectral family and let us put $(\hat{E}_Q(\alpha)f)(x) = g(\alpha, x)$. The spectral resolution of $\hat{Q}$ requires that

$$xf(x) = (\hat{Q}f)(x) = \int_{-\infty}^{\infty} \alpha \, d\hat{E}_Q(\alpha)f)(x) = \int_{-\infty}^{\infty} \alpha \, dg(\alpha, x) \tag{2.286}$$

A solution of this equation is obtained if we set $dg(\alpha, x) = \delta(\alpha - x) f(x)\, d\alpha$. We then get

$$\begin{aligned} \hat{E}_Q(\alpha) f)(x) = g(\alpha, x) &= \int_{-\infty}^{\alpha} dg(\alpha', x) \\ &= \int_{-\infty}^{\alpha} \delta(\alpha' - x) f(x)\, d\alpha' = \chi(\alpha - x) f(x) \end{aligned} \tag{2.287}$$

where $\chi(\alpha - x)$ is the Heaviside function

$$\chi(x) = \begin{cases} +1 & \text{if} \quad 0 \leq x \\ 0 & \text{if} \quad 0 > x \end{cases} \tag{2.288}$$

According to this calculation $\hat{E}_Q(\alpha)$ is the multiplicative operator $\chi(\alpha - x)$ as above.

We now need to verify that the solution we have constructed gives the unique spectral family belonging to $\hat{Q}$.

First we show that the solution is a spectral family, that is, that it has the properties(on page 50) required by the definition given earlier. Since the $\hat{E}_Q(\alpha)$ are multiplicative operators, it is clear that they commute. Property (1) is equivalent to

$$\hat{E}(\alpha)\hat{E}(\alpha') = \hat{E}(\alpha) \quad , \quad \alpha \leq \alpha' \tag{2.289}$$

a property that is clearly satisfied by the multiplicative operator $\chi(\alpha - x)$. Property (2) holds because $\chi(x)$ was defined to be continuous on the right, while properties (3) are clear.

Next we have to verify that the spectral family found does in fact belong to $\hat{Q}$. According to the spectral theorem we must have

$$\langle f | \hat{Q} | g \rangle = \int_{-\infty}^{\infty} \alpha \, d \langle f | \hat{E}_Q(\alpha) | g \rangle \tag{2.290}$$

or

$$\int_{-\infty}^{\infty} f^*(x) x g(x)\, dx = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} d\alpha\, f^*(x)\delta(\alpha - x)g(x) \tag{2.291}$$

which is clearly true by definition of the δ-function.

The spectral family $\hat{E}_Q(\alpha)$ is continuous everywhere and increasing in $(-\infty, \infty)$. The spectrum of $\hat{Q}$ consists therefore of the whole of the real axis and is pure continuous. The projection $\hat{E}_Q[\Delta]$ is the *characteristic function* $\chi(\Delta)$ of the interval Δ, that is, a function of x equal to one if $x \in \Delta$ and zero otherwise.

Some final thoughts about these ideas.....

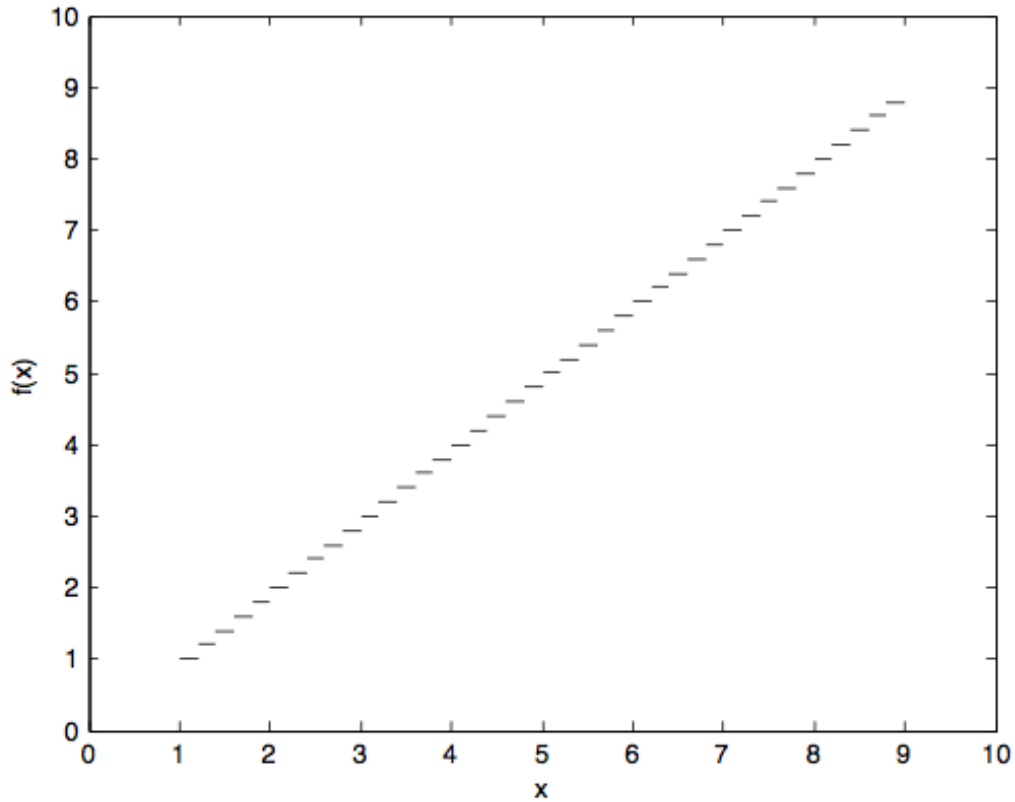
Projection Operators and Continuous Spectra - An Example

In the macroscopic world, if we want to locate the position of an object, we use a calibrated ruler. Formally, the physical position x is a continuous variable.

The ruler, however, only has a finite resolution. An outcome anywhere within the j^{th} interval is said to correspond to the value x_j. Thus, effectively, the result of the position measurement is not the original continuous variable x, but rather a staircase function,

$$x' = f(x) = x_j \quad , \quad \forall \quad x_j \leq x \leq x_{j+1} \tag{2.292}$$

as illustrated in the figure below of the "staircase function".



These considerations are easily translated in quantum language.

In the x-representation, an operator x' is defined as multiplication by the staircase function $f(x)$. This operator has a finite number of discrete eigenvalues x_j. Each one of the eigenvalues is infinitely degenerate, that is, any state vector with domain between x_j and x_{j+1} falls entirely within the j^{th} interval of the ruler (see Figure 4.1), and therefore corresponds to the degenerate eigenvalue x_j.

Orthogonal resolution of the Identity

An experimental setup for a quantum test described by the above formalism could have, at its final stage, an array of closely packed detectors, labeled by the real numbers x_j. Such a quantum test thus asks, simultaneously, a set of questions

$$\text{Is} \quad x_j \leq x \leq x_{j+1} \quad ? \tag{2.293}$$

(one question for each j).

The answers, *yes* and *no*, can be give numerical values 0 and 1, respectively. Each of these questions therefore corresponds to the operator $\hat{P}_j$, which is itself a function of x:

$$\hat{P}_j(x) = \begin{cases} 1 & \text{if} \quad x_j \leq x \leq x_{j+1} \\ 0 & \text{otherwise} \end{cases} \tag{2.294}$$

Clearly, these operators satisfy

$$\hat{P}_j \hat{P}_k = \delta_{jk} \hat{P}_k \quad \textit{and} \quad \sum_j \hat{P}_j = \hat{I} \tag{2.295}$$

This implies that they are projection operators (or projectors) and the questions will correspond to the *measurement* of the projection operators.

The staircase function $x' = f(x)$ defined above can then be written as

$$x' = \sum_j s_j \hat{P} \tag{2.296}$$

This operator x' approximates the operator x as well as is allowed by the finite resolution of the ruler.

How do we proceed to the continuum limit? Let us define a *spectral family* of operators

$$\hat{E}(x_j) = \sum_{k=0}^{j-1} \hat{P}_k \tag{2.297}$$

They obey the recursion relations

$$\hat{E}(x_{j+1}) = \hat{E}(x_j) + \hat{P}_j \tag{2.298}$$

and the boundary conditions

$$\hat{E}(x_{min}) = 0 \quad , \quad \hat{E}(x_{max}) = \hat{I} \tag{2.299}$$

The physical meaning of the operator $\hat{E}(x_j)$ is the question

$$''Is \quad x \leq x_j \quad ?'' \tag{2.300}$$

with answers yes $= 1$ and no $= 0$.

We then have

$$\begin{aligned} \hat{E}(x_j)\hat{E}(x_m) &= \sum_{k=0}^{j-1} \hat{P}_k \sum_{n=0}^{m-1} \hat{P}_n = \sum_{k=0}^{j-1} \sum_{n=0}^{m-1} \hat{P}_k \hat{P}_n \\ &= \sum_{k=0}^{j-1} \sum_{n=0}^{m-1} \delta_{kn} \hat{P}_n = \begin{cases} \hat{E}(x_j) & \text{if} \quad x_j \leq x_m \\ \hat{E}(x_m) & \text{if} \quad x_m \leq x_j \end{cases} \end{aligned} \tag{2.301}$$

so that the $\hat{E}(x_j)$ are projectors.

We can now pass to the continuum limit. We define $\hat{E}(\xi)$ as the projector which represents the question

$$''Is \quad x \leq \xi \quad ?'' \tag{2.302}$$

and which returns, as the answer, a numerical value(yes = 1, no = 0). We then consider two neighboring values, ξ and $\xi + d\xi$, and define an *infinitesimal* projector,

$$d\hat{E}(\xi) = \hat{E}(\xi + d\xi) - \hat{E}(\xi) \tag{2.303}$$

which represents the question "Is $\xi \leq x \leq \xi + d\xi$?". This $d\hat{E}(\xi)$ thus behaves as an infinitesimal increment $\hat{P}_j$ in the equation

$$\hat{E}(x_{j+1}) = \hat{E}(x_j) + \hat{P}_j \tag{2.304}$$

We then have, instead of the staircase approximation, the exact result

$$x = \int_0^1 \xi \, d\hat{E}(\xi) \tag{2.305}$$

Note that the integration limits are actually operators, namely, $\hat{E}(x_{min}) = 0$ and $\hat{E}(x_{max}) = 1$.

This equation is the *spectral decomposition* or *spectral resolution* of the operator x and the operators $\hat{E}(\xi)$ are the *spectral family* (or *resolution of the identity*) generated by x. We can now define any function of the operator x

$$f(x) = \int_0^1 f(\xi)\, d\hat{E}(\xi) \tag{2.306}$$

Note that the right hand sides of the last two equations are Stieltjes integrals.

If we consider a small increment $d\xi \to 0$, then the limit $d\hat{E}(\xi)/d\xi$ exists and the integration step can be taken as the c-number $d\xi$ rather than $d\hat{E}(\xi)$, which is an operator. We then have an operator valued Riemann integral

$$\int_0^1 f(\xi)\, d\hat{E}(\xi) = \int_{x_{min}}^{x_{max}} f(\xi) \frac{d\hat{E}(\xi)}{d\xi}\, d\xi \tag{2.307}$$

This type of spectral decomposition applies not only to operators with continuous spectra, but also to those having discrete spectra, or even mixed spectra.

For a discrete spectrum, $d\hat{E}(\xi) = 0$ if ξ lies between consecutive eigenvalues, and $d\hat{E}(\xi) = \hat{P}_k$, that is, the projector on the k^{th} eigenstate, if the k^{th} eigenvalue lies between ξ and $\xi + d\xi$.

The projector $\hat{E}(\xi)$ is a bounded operator, which depends on the parameter ξ. It may be a discontinuous function of ξ, but it never is infinite, and we never actually need $d\hat{E}(\xi)/d\xi$. This is the advantage of the Stieltjes integral over the more familiar Riemann integral: the left-hand side of the last equation is always meaningful, even if the the right-hand side is not.

Some Useful Properties

If $f(\xi)$ is a real function, then $f(x)$ is given by

$$f(x) = \int_0^1 f(\xi)\, d\hat{E}(\xi) \tag{2.308}$$

is a self-adjoint operator.

We also have

$$\int f(\xi)\, d\hat{E}(\xi) \int g(\eta)\, d\hat{E}(\eta) = \int f(\zeta) g(\zeta)\, d\hat{E}(\zeta) \tag{2.309}$$

$$e^{if(x)} = \int e^{if(\xi)}\, d\hat{E}(\xi) \tag{2.310}$$

The spectral decomposition of a self-adjoint operator will allow us to give a rigorous definition of the measurement of a continuous variable. It will be equivalent to an infinite set of yes-no questions where each question is represented by a bounded(but infinitely degenerate) projection operator.

Looking ahead to quantum mechanics .....

An operator such as $\hat{Q}$ that has a continuous spectrum is said to have a *formal* eigenvalue equation in Dirac language

$$\hat{Q}\,|q\rangle = q\,|q\rangle \tag{2.311}$$

In the development of the theory, we will make assumptions that will lead to the orthonormality condition for the continuous case taking the form

$$\langle q' \,|\, q'' \rangle = \delta(q' - q'') \tag{2.312}$$

Since this implies that $\langle q \,|\, q \rangle = \infty$, these formal eigenvectors have infinite norm. Thus, the Dirac formulation that we will construct for operators with a continuous spectrum will not fit into the mathematical theory of Hilbert space, which admits only vectors of finite norm.

Operators will take the form

$$\hat{Q} = \int_{-\infty}^{\infty} q \, |q\rangle \, \langle q| \, dq \tag{2.313}$$

which is the continuous analog of our earlier expressions.

The projection operator will be formally given by

$$\hat{E}_\beta = \int_{-\infty}^{\beta} |q\rangle \, \langle q| \, dq \tag{2.314}$$

It is well-defined in Hilbert space, but its derivative

$$\frac{d\hat{E}_\beta}{dq} = |q\rangle \, \langle q| \tag{2.315}$$

does not exist within the Hilbert space framework.

There are two alternative methods for making quantum mechanics fit within a mathematically rigorous Hilbert space framework. The first would be to restrict or revise the formalism to make it fit(still not admit states of infinite norm). The second would be to extend the Hilbert space so that vectors of infinite norm are allowed. We will discuss these ideas later and make appropriate choices.

We saw earlier in the finite-dimensional case, where we have a discrete spectrum of eigenvalues, that the value of the projection operator $\hat{E}_x$ for the operator $\hat{B}$ jumped by $\hat{P}_k = |b_k\rangle \langle b_k|$ as x passed through the k^{th} eigenvalue b_k.

For the infinite dimensional case, where we can have both a discrete and a continuous spectrum of eigenvalues, the projection operator behaves in the same way as we move about the discrete part of the spectrum. In the continuous part of the spectrum, however, it is possible for the projection operator to exhibit a continuous increase in value.

In a more formal manner we state: if $\hat{B}$ is a self-adjoint operator and $\hat{E}_x$ is the projection operator of its spectral decomposition, then

1. the set of points x on which $\hat{E}_x$ increases is called the *spectrum* of $\hat{B}$; alternatively, a point is in the spectrum if it is not in an interval on which $\hat{E}_x$ is constant.
2. the set of points x on which $\hat{E}_x$ jumps is called the point spectrum of $\hat{B}$; the point spectrum is the set of all eigenvalues.
3. the set of points x on which $\hat{E}_x$ increases continuously is called the *continuous spectrum* of $\hat{B}$.
4. the point spectrum and the continuous spectrum comprise the total spectrum.

In quantum mechanics, as we shall see, a real physical, measurable quantity will be represented by a self-adjoint operator. The spectrum of the operator will be the set of real numbers that correspond to the possible measured values of the physical quantity.

The projection operators in the spectral decomposition will be used to describe the probability distributions of these values and the state operators. We will get discrete probability distributions over the point spectrum and continuous probability distributions over the continuous spectrum.

All of these new mathematical quantities will have direct and important physical meaning!

2.19 **Functions of Operators (general case); Stone's Theorem**

We mentioned earlier that functions of operators also have a decomposition into projection operators. In fact, we wrote

$$g(\hat{B}) = \int_{-\infty}^{\infty} g(x)\, d\hat{E}_x \tag{2.316}$$

The ability to deal with functions of operators will be very important in quantum mechanics, so let us spend more time looking at the mathematical details involved.

for all vectors $|\alpha\rangle$ and $|\beta\rangle$. Now a self-adjoint operator is bounded if and only if its spectrum is bounded. If $f(\hat{B})$ is a bounded operator on the spectrum of $\hat{B}$, then it turns out that the above equation for all $|\alpha\rangle$ and $|\beta\rangle$ defines $f(\hat{B})\,|\eta\rangle$ for all vectors $|\eta\rangle$.

Is the above definition reasonable? We can see that it is by looking at some properties and some simple examples.

Let $f(x) = x$. This implies that $f(\hat{B}) = \hat{B}$ since we must have

$$\langle\alpha|\,\hat{B}\,|\beta\rangle = \int_{-\infty}^{\infty} x\,d\,\langle\alpha|\,\hat{E}_x\,|\beta\rangle \tag{2.319}$$

$$\langle\alpha|\,\hat{I}\,|\beta\rangle = \int_{-\infty}^{\infty} d\,\langle\alpha|\,\hat{E}_x\,|\beta\rangle = \langle\alpha\,|\,\beta\rangle \tag{2.320}$$

If we let

$$(f+g)(x) = f(x) + g(x) \tag{2.321}$$

$$(cf)(x) = cf(x) \tag{2.322}$$

we then have

$$(f+g)(\hat{B}) = f(\hat{B}) + g(\hat{B}) \tag{2.323}$$

$$(cf)(\hat{B}) = cf(\hat{B}) \tag{2.324}$$

so that sums and multiples of functions of operators are defined in a standard way.

If we let

$$(fg)(x) = f(x)g(x) \tag{2.325}$$

we then have

$$\begin{aligned}
\langle\alpha|\, f(\hat{B})g(\hat{B})\,|\beta\rangle &= \int_{-\infty}^{\infty} f(x)\, d\,\langle\alpha|\, \hat{E}_x g(\hat{B})\,|\beta\rangle \\
&= \int_{-\infty}^{\infty} f(x)\, d_x \int_{-\infty}^{\infty} g(y)\, d_y\, \langle\alpha|\, \hat{E}_x \hat{E}_y\,|\beta\rangle \\
&= \int_{-\infty}^{\infty} f(x)\, d \int_{-\infty}^{x} g(y)\, d\,\langle\alpha|\, \hat{E}_y\,|\beta\rangle \\
&= \int_{-\infty}^{\infty} f(x)g(x)\, d\,\langle\alpha|\, \hat{E}_x\,|\beta\rangle \\
&= \int_{-\infty}^{\infty} (fg)(x)\, d\,\langle\alpha|\, \hat{E}_x\,|\beta\rangle = \langle\alpha|\, (fg)(\hat{B})\,|\beta\rangle
\end{aligned} \tag{2.326}$$

so that

$$(fg)(\hat{B}) = f(\hat{B})g(\hat{B}) \tag{2.327}$$

as it should. We can also show that $f(\hat{B})g(\hat{B}) = g(\hat{B})f(\hat{B})$ so that all functions of the operator $\hat{B}$ commute.

With these properties, we can then define a polynomial function of an operator by

$$f(x) = c_0 + c_1 x + c_2 x^2 + \ldots + c_n x^n \tag{2.328}$$

$$f(\hat{B}) = c_0 + c_1 \hat{B} + c_2 \hat{B}^2 + \ldots + c_n \hat{B}^n \tag{2.329}$$

for any vectors $|\alpha\rangle$ and $|\beta\rangle$.

Thus, products of functions of operators are also defined in the standard way.

If we let $(f^*)(x) = f^*(x)$, then for any vectors $|\alpha\rangle$ and $|\beta\rangle$ we have

$$\begin{aligned}\langle\alpha| \left[f(\hat{B})\right]^* |\beta\rangle &= \langle\beta| f(\hat{B}) |\alpha\rangle^* \\ &= \int_{-\infty}^{\infty} f^*(x)\, d\langle\alpha| \hat{E}_x |\beta\rangle = \int_{-\infty}^{\infty} (f^*)(x)\, d\langle\alpha| \hat{E}_x |\beta\rangle\end{aligned} \tag{2.330}$$

or

$$\left[f(\hat{B})\right]^* = (f^*)(\hat{B}) \tag{2.331}$$

If $f(x)$ is a real function, this implies that $f(\hat{B})$ is also a self-adjoint operator.

If $f^* f = 1$, then $f(\hat{B})$ is a unitary operator since

$$\left[f(\hat{B})\right]^\dagger f(\hat{B}) = \hat{I} = f(\hat{B}) \left[f(\hat{B})\right]^\dagger \tag{2.332}$$

Now for any vector $|\alpha\rangle$ we have

$$\begin{aligned} \langle\alpha| f(\hat{B}) |\alpha\rangle &= \int_{-\infty}^{\infty} f(x)\, d \langle\alpha| \hat{E}_x |\alpha\rangle \\ &= \int_{-\infty}^{\infty} f(x)\, d \langle\alpha| \hat{E}_x \hat{E}_x |\alpha\rangle = \int_{-\infty}^{\infty} f(x)\, d \| \hat{E}_x |\alpha\rangle \|^2 \end{aligned} \tag{2.333}$$

If we define a self-adjoint operator to be positive if and only if it spectrum is non-negative, then $f(\hat{B})$ is positive if $f(x)$ is non-negative over the spectrum of $\hat{B}$ and $f(\hat{B})$ is bounded if $|f(x)|$ is bounded over the spectrum of $\hat{B}$.

In the special case where $\hat{B}$ has only a point spectrum, we have

$$\hat{B} = \sum_k b_k \hat{P}_k \tag{2.334}$$

and then for any vectors $|\alpha\rangle$ and $|\beta\rangle$

$$\begin{aligned} \langle\alpha| f(\hat{B}) |\beta\rangle &= \langle\alpha| f\left(\sum_k b_k \hat{P}_k\right) |\beta\rangle = \sum_k \langle\alpha| f(b_k \hat{P}_k) |\beta\rangle \\ &= \sum_k f(b_k) \langle\alpha| \hat{P}_k |\beta\rangle = \langle\alpha| \sum_k f(b_k) \hat{P}_k |\beta\rangle \end{aligned} \tag{2.335}$$

or

$$f(\hat{B}) = \sum_k f(b_k) \hat{P}_k \tag{2.336}$$

as we expected.

We define the same properties for unitary operator. Let

$$\hat{U} = \int_0^{2\pi} e^{ix}\, d\hat{E}_x \tag{2.337}$$

and also let

$$\langle\alpha|\, \hat{B}\, |\beta\rangle = \int_0^{2\pi} x\, d\, \langle\alpha|\, \hat{E}_x\, |\beta\rangle \tag{2.338}$$

for all vectors in the space.

This defines a bounded self-adjoint operator $\hat{B}$ with spectral decomposition

$$\hat{B} = \int_0^{2\pi} x\, d\hat{E}_x \tag{2.339}$$

We then have

$$\langle\alpha|\, \hat{U}\, |\beta\rangle = \int_0^{2\pi} e^{ix}\, d\, \langle\alpha|\, \hat{E}_x\, |\beta\rangle = \int_0^{2\pi} f(x)\, d\, \langle\alpha|\, \hat{E}_x\, |\beta\rangle = \langle\alpha|\, f(\hat{B})\, |\beta\rangle \tag{2.340}$$

which implies that $\hat{U}$, in this case, must be a particular function of $\hat{B}$, namely $\hat{U} = e^{i\hat{B}}$. In addition, any function of $\hat{U}$ is clearly a function of $\hat{B}$.

There exists another relation between Hermitian and unitary operators that is a fundamental property in quantum mechanics. Let $\hat{H}$ be a self-adjoint operator with the spectral decomposition

$$\hat{H} = \int_{-\infty}^{\infty} x \, d\hat{E}_x \tag{2.341}$$

For every real number t let

$$\langle\alpha| \hat{U}_t |\beta\rangle = \int_0^{2\pi} e^{itx} \, d \langle\alpha| \hat{E}_x |\beta\rangle \tag{2.342}$$

This then defines an operator $\hat{U}_t = e^{it\hat{H}}$ which is unitary since $(e^{itx})^* e^{itx} = 1$. We also have $\hat{U}_0 = \hat{I}$.

Now since

$$e^{itx}e^{it'x} = e^{i(t+t')x} \tag{2.343}$$

we must have

$$\hat{U}_t\hat{U}_{t'} = \hat{U}_{t+t'} \tag{2.344}$$

for all real numbers t and t'.

The converse of this property is called *Stone's theorem*:

For each real number t let $\hat{U}_t$ be a unitary operator. Assume that $\langle\alpha|\,\hat{U}_t\,|\beta\rangle$ is a continuous function of t for all vectors $|\alpha\rangle$ and $|\beta\rangle$. If $\hat{U}_0 = \hat{I}$ and $\hat{U}_t\hat{U}_{t'} = \hat{U}_{t+t'}$ for all real numbers t and t', then there is a unique self-adjoint operator $\hat{H}$ such that $\hat{U}_t = e^{it\hat{H}}$ for all t. A vector $|\beta\rangle$ is in the domain of $\hat{H}$ if and only if the vectors

$$\frac{1}{it}(\hat{U}_t - \hat{I})\,|\beta\rangle \tag{2.345}$$

converge to a limit as $t \to 0$.

The limit vector is $\hat{H}\,|\beta\rangle$. If a bounded operator commutes with $\hat{U}_t$, then it commutes with $\hat{H}$.

This theorem leads to the following very important result.

If $\hat{U}_t\,|\beta\rangle$ is in the domain of $\hat{H}$, then

$$\frac{1}{i\Delta t}(\hat{U}_{\Delta t} - \hat{I})\hat{U}_t\,|\beta\rangle \to \hat{H}\hat{U}_t\,|\beta\rangle \tag{2.346}$$

or

$$\frac{1}{i\Delta t}(\hat{U}_{\Delta t}\hat{U}_t - \hat{U}_t)\,|\beta\rangle = \frac{1}{i\Delta t}(\hat{U}_{t+\Delta t} - \hat{U}_t)\,|\beta\rangle \to -i\frac{d}{dt}\hat{U}_t\,|\beta\rangle \tag{2.347}$$

as $\Delta t \to 0$.

We can then write

$$-i\frac{d}{dt}\hat{U}_t\,|\beta\rangle = \hat{H}\hat{U}_t\,|\beta\rangle \tag{2.348}$$

This equation will eventually tell us how the physical states(ket vectors) and state operators that will represent physical systems evolve in time (it will lead to the Schrodinger equation, which is the time evolution equation in one representation of quantum mechanics).

Examples - Functions of Operators

Suppose that we have the eigenvector/eigenvalue equations for a self-adjoint operator

$$\hat{A}\,|k\rangle = a_k\,|k\rangle \quad , \quad k = 1, 2, \ldots, N \tag{2.349}$$

We then *assume* that

$$f(\hat{A})\,|k\rangle = f(a_k)\,|k\rangle \quad , \quad k = 1, 2, \ldots, N \tag{2.350}$$

for the eigenvectors.

We can show that this works for polynomials and power series as follows:

$$|\psi\rangle = \sum_{k=1}^{N} |k\rangle \langle k \,|\, \psi\rangle \tag{2.351}$$

$$\begin{aligned} \hat{A}\,|\psi\rangle &= \hat{A} \sum_{k=1}^{N} |k\rangle \langle k \,|\, \psi\rangle = \sum_{k=1}^{N} \hat{A}\,|k\rangle \langle k \,|\, \psi\rangle \\ &= \sum_{k=1}^{N} a_k\,|k\rangle \langle k \,|\, \psi\rangle = \left(\sum_{k=1}^{N} a_k\,|k\rangle \langle k| \right) |\psi\rangle \end{aligned} \tag{2.352}$$

$$\rightarrow \hat{A} = \sum_{k=1}^{N} a_k\,|k\rangle \langle k| \rightarrow \text{ spectral resolution of the operator} \tag{2.353}$$

Now define the *projection* operator

$$\hat{P}_k = |k\rangle \langle k| \rightarrow \hat{P}_k \hat{P}_j = \hat{P}_k \delta_{kj} \tag{2.354}$$

We then have

$$\hat{A} = \sum_{k=1}^{N} a_k \left|k\right\rangle \left\langle k\right| = \sum_{k=1}^{N} a_k \hat{P}_k \tag{2.355}$$

or any operator is represented by a sum over its eigenvalues and corresponding projection operators.

We then have

$$\begin{aligned} \hat{A}^2 &= \left(\sum_{k=1}^{N} a_k \hat{P}_k \right) \left(\sum_{j=1}^{N} a_j \hat{P}_j \right) = \sum_{k,j=1}^{N} a_k a_j \hat{P}_k \hat{P}_j \\ &= \sum_{k,j=1}^{N} a_k a_j \hat{P}_k \delta_{kj} = \sum_{k=1}^{N} a_k^2 \hat{P}_k \rightarrow \hat{A}^n = \sum_{k=1}^{N} a_k^n \hat{P}_k \end{aligned} \tag{2.356}$$

Therefore, for

$$f(x) = \sum_{n=1}^{N} q_n x^n \tag{2.357}$$

we have

$$f(\hat{A}) = \sum_{n=1}^{N} q_n \hat{A}^n = \sum_{n=1}^{N} q_n \sum_{k=1}^{N} a_k^n \hat{P}_k$$
$$= \sum_{k=1}^{N} \left(\sum_{n=1}^{N} q_n a_k^n \right) \hat{P}_k = \sum_{k=1}^{N} f(a_k) \hat{P}_k \tag{2.358}$$

This says that, in general, we have

$$f(\hat{A}) \left| \psi \right\rangle = f(\hat{A}) \sum_{k=1}^{N} \left| k \right\rangle \left\langle k \right| \psi \rangle = \sum_{k=1}^{N} f(\hat{A}) \left| k \right\rangle \left\langle k \right| \psi \rangle$$
$$= \sum_{k=1}^{N} f(a_k) \left| k \right\rangle \left\langle k \right| \psi \rangle = \left(\sum_{k=1}^{N} f(a_k) \left| k \right\rangle \left\langle k \right| \right) \left| \psi \right\rangle \tag{2.359}$$

$$\rightarrow f(\hat{A}) = \sum_{k=1}^{N} f(a_k)^n \left| k \right\rangle \left\langle k \right| \rightarrow \text{ spectral resolution of the operator} \tag{2.360}$$

Numerical example: consider the operator

$$\hat{A} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix}$$

which has eigenvalues 7 and 1 with eigenvectors

$$|7\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad , \qquad |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

This gives

$$\hat{P}_7 = |7\rangle \langle 7| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad , \qquad \hat{P}_1 = |1\rangle \langle 1| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

and therefore

$$\hat{A} = 7\hat{P}_7 + \hat{P}_1 = \frac{7}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix}$$

$$\hat{A}^2 = 7^2\hat{P}_7 + \hat{P}_1 = \frac{49}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$$

$$= \begin{pmatrix}25 & 24\\ 24 & 25\end{pmatrix} = \begin{pmatrix}4 & 3\\ 3 & 4\end{pmatrix}\begin{pmatrix}4 & 3\\ 3 & 4\end{pmatrix}$$

$$\log\left(\hat{A}\right) = \log(7)\hat{P}_7 + \log(1)\hat{P}_1 = \frac{\log(7)}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}$$

$$\sqrt{\hat{A}} = \sqrt{7}\hat{P}_7 + \hat{P}_1 = \frac{\sqrt{7}}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix}\sqrt{7}+1 & \sqrt{7}-1\\ \sqrt{7}-1 & \sqrt{7}+1\end{pmatrix}$$

Clearly we then have

$$\log\left(\hat{A}\right)|7\rangle = \frac{\log(7)}{2\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1\\ 1\end{pmatrix} = \frac{\log(7)}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix} = \log(7)|7\rangle$$

$$\log\left(\hat{A}\right)|1\rangle = \frac{\log(7)}{2\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1\\ -1\end{pmatrix} = \frac{\log(7)}{2\sqrt{2}}\begin{pmatrix}0\\ 0\end{pmatrix} = 0 = \log(1)|1\rangle$$

as expected.

The big question that remains is then

$$\text{Is} \quad \hat{f}(\hat{A}) = f(\hat{A}) \; ? \tag{2.361}$$

no proof exists!

2.20 **Commuting Operators**

As we stated earlier, the commutator of two operators is given by

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{2.362}$$

If $\hat{A}$ and $\hat{B}$ are self-adjoint operators, each possessing a complete set of eigenvectors, and if they commute, then there exists a complete set of vectors which are eigenvectors of both $\hat{A}$ and $\hat{B}$, that is, they possess a common set of eigenvectors.

This theorem extends to any number of commuting operators. If we have a set of N mutually commuting operators, then they all have a common set of eigenvectors.

The reverse is also true. If two operators possess a common set of eigenvectors, then they commute.

Let $\{\hat{A}, \hat{B}, \hat{C}, \ldots\}$ be a set of mutually commuting operators that possess a complete set of common eigenvectors. Corresponding to a particular eigenvalue for each operator, there may be more than one eigenvector. If, however, there is no more than one eigenvector for each set of eigenvalues $(a_k, b_k, c_k, \ldots)$, then the operators $\{\hat{A}, \hat{B}, \hat{C}, \ldots\}$ are said to be a complete commuting set of operators.

Any operator that commutes with all members of a complete commuting set must be a function of the operators in that set.

Let us now think about these ideas in terms of projection operators.

Let $\hat{Q}$ be a Hermitian operator with a pure point spectrum so that we can write

$$\hat{Q} = \sum_k q_k \hat{P}_k \tag{2.363}$$

where each q_k is a *different* eigenvalue of $\hat{Q}$ and $\hat{P}_k$ is the projection operator onto the subspace corresponding to eigenvalue q_k.

Let $\hat{R}$ be a bounded Hermitian operator that commutes with $\hat{Q}$. For each k and for any arbitrary vector $|\eta\rangle$ we then have

$$\begin{aligned}\hat{Q}\hat{R}\hat{P}_k\,|\eta\rangle = \hat{R}\hat{Q}\hat{P}_k\,|\eta\rangle &= \hat{R}\left(\sum_j q_j \hat{P}_j\right)\hat{P}_k\,|\eta\rangle \\ &= \hat{R}\sum_j q_j \delta_{jk}\hat{P}_k\,|\eta\rangle = q_k\hat{R}\hat{P}_k\,|\eta\rangle \end{aligned} \tag{2.364}$$

where we have used the relation

$$\hat{P}_j \hat{P}_k = \delta_{jk} \hat{P}_k \tag{2.365}$$

for any vector $|\eta\rangle$. Thus, $\hat{R}\hat{P}_k |\eta\rangle$ is an eigenvector of $\hat{Q}$ with eigenvalue q_k. Therefore, $\hat{P}_k \hat{R} \hat{P}_k |\eta\rangle = \hat{R}\hat{P}_k |\eta\rangle$ for all $|\eta\rangle$ and we have

$$\hat{R}\hat{P}_k = \hat{P}_k \hat{R} \hat{P}_k \tag{2.366}$$

Taking the adjoint of both sides we get

$$\left(\hat{R}\hat{P}_k\right)^\dagger = \left(\hat{P}_k \hat{R} \hat{P}_k\right)^\dagger \tag{2.367}$$

$$\hat{R}\hat{P}_k = \hat{P}_k \hat{R} \hat{P}_k \tag{2.368}$$

Thus,

$$\hat{R}\hat{P}_k = \hat{P}_k \hat{R} \tag{2.369}$$

or *each* $\hat{P}_k$ commutes with every bounded Hermitian operator which commutes with $\hat{Q}$.

We can extend this result to operators possessing both a point and continuous spectrum. If $\hat{Q}$ is a self-adjoint operator with the spectral decomposition

$$\hat{Q} = \int_{-\infty}^{\infty} x \, d\hat{E}_x \tag{2.370}$$

and if $\hat{R}$ is a bounded self-adjoint operator that commutes with $\hat{Q}$, then

$$\hat{E}_x \hat{R} = \hat{R} \hat{E}_x \tag{2.371}$$

for every x.

Let us now express the ideas of complete commuting sets in terms of projection operators.

Let $\{\hat{B}_1, \hat{B}_2, \ldots, \hat{B}_N\}$ be a set of mutually commuting Hermitian operators with pure point spectra. For each we then have

$$\hat{B}_r = \sum_k b_k^{(r)} \hat{P}_k^{(r)} \quad , \quad r = 1, 2, \ldots, N \tag{2.372}$$

where each $b_k^{(r)}$ is a different eigenvalue of $\hat{B}_r$ and $\hat{P}_k^{(r)}$ is the projection operator onto the subspace spanned by the eigenvectors of $\hat{B}_r$ corresponding to $b_k^{(r)}$.

By definition then, the projection operators $\hat{P}_k^{(r)}$ commute with each other for all different r and k

$$\hat{P}_j^{(r)} \hat{P}_k^{(s)} = \hat{P}_k^{(s)} \hat{P}_j^{(r)} \tag{2.373}$$

This implies that

$$\hat{P}_i^{(1)} \hat{P}_j^{(2)} \ldots \hat{P}_l^{(N)} \tag{2.374}$$

is the projection operator for any $i, j, \ldots, N$, that is, it projects onto the subspace of all vectors $|\alpha\rangle$ such that

$$\hat{B}_1 |\alpha\rangle = b_i^{(1)} |\alpha\rangle \ , \ \hat{B}_2 |\alpha\rangle = b_j^{(2)} |\alpha\rangle \ , \ \ldots \ , \ \hat{B}_N |\alpha\rangle = b_l^{(N)} |\alpha\rangle \tag{2.375}$$

These projection operators are mutually orthogonal

$$\hat{P}_i^{(1)} \hat{P}_j^{(2)} \ldots \hat{P}_l^{(N)} \hat{P}_{i'}^{(1)} \hat{P}_{j'}^{(2)} \ldots \hat{P}_{l'}^{(N)} = \delta_{ii'} \delta_{jj'} \ldots \delta_{ll'} \hat{P}_i^{(1)} \hat{P}_j^{(2)} \ldots \hat{P}_l^{(N)} \tag{2.376}$$

and they have the completeness property that

$$\sum_i \sum_j \ldots \sum_l \hat{P}_i^{(1)} \hat{P}_j^{(2)} \ldots \hat{P}_l^{(N)} = \hat{I} \tag{2.377}$$

Note that some of these projection operators might be zero.

Suppose that none of them projects onto a subspace of dimension larger than one.

In this case, we say that the set of operators $\{\hat{B}_1, \hat{B}_2, \ldots, \hat{B}_N\}$ is a *complete set of commuting operators.*

Now let us return to the study of a continuous spectrum.

First, we repeat some earlier material to set the stage.

Let us start with a very simple example so we can figure out how to proceed and then generalize to a more complicated case. We consider the space $L^2(-\infty, \infty)$ and a single Hermitian operator $\hat{Q}$ defined by

$$(\hat{Q}g)(x) = xg(x) \tag{2.378}$$

It turns out that every bounded operator which commutes with $\hat{Q}$ is a function of $\hat{Q}$.

Now, there exists a theorem: Suppose we have a set of mutually commuting operators $\{\hat{A}_i\}$.

This is a complete set of commuting operators if an only if every bounded operator which commutes with all $\{\hat{A}_i\}$ is a function of the $\{\hat{A}_i\}$.

In the previous discussion, we had the case of a complete commuting set consisting of a single operator.

The spectrum of $\hat{Q}$ is purely continuous and consists of all real numbers x. Each vector g is a function $g(x)$ on the spectrum of $\hat{Q}$.

We connect this to the case of a complete set of commuting operators with a pure point spectra as follows.

We define two abstract vectors $|x\rangle$ and $|g\rangle$ such that

$$\langle x \,|\, g \rangle = g(x) \tag{2.379}$$

We then have

$$(\hat{Q}g)(x) = \left\langle x \,\middle|\, \hat{Q}g \right\rangle = x \,\langle x \,|\, g \rangle = xg(x) \tag{2.380}$$

which is the spectral representation of $\hat{Q}$. We can generalize to a function of $\hat{Q}$ with

$$\left\langle x \left| f(\hat{Q})g \right\rangle = f(x) \left\langle x \,|\, g \right\rangle = f(x)g(x) \tag{2.381}$$

In Dirac language, we write an abstract equation like

$$\hat{Q} \left| x \right\rangle = x \left| x \right\rangle \tag{2.382}$$

We then have

$$x^* \left\langle x \right| = x \left\langle x \right| = \left\langle x \right| \hat{Q}^\dagger = \left\langle x \right| \hat{Q} \tag{2.383}$$

and

$$\left\langle x \right| \hat{Q} \left| g \right\rangle = x \left\langle x \,|\, g \right\rangle = xg(x) \tag{2.384}$$

which again gives the spectral representation of $\hat{Q}$.

Finally we have

$$\langle x|\, f(\hat{Q})\, |g\rangle = f(x)\, \langle x\,|\, g\rangle = f(x)g(x) \tag{2.385}$$

The problem with defining an abstract Hermitian operator $\hat{Q}$ by

$$\hat{Q}\, |x\rangle = x\, |x\rangle \tag{2.386}$$

is that $\hat{Q}$ has no eigenvectors in the Hilbert space L^2 of square-integrable functions. In order for there to be eigenvectors we must have

$$(\hat{Q}g)(x) = \hat{Q}g(x) = xg(x) = ag(x) \tag{2.387}$$

for a real number a.

This implies that $g(x)$ is zero for all points $x \neq a$ and

$$\|g\|^2 = \int_{-\infty}^{\infty} |g|^2 = 0 \tag{2.388}$$

because the *standard* integral is not changed by the value of the integrand at a *single point*.

Now we have

$$\langle x|\,\hat{Q}\,|a\rangle = x\,\langle x\,|\,a\rangle = a\,\langle x\,|\,a\rangle \tag{2.389}$$

If we replace the inner product by

$$\langle x\,|\,a\rangle = \langle a\,|\,x\rangle = \delta(x-a) \tag{2.390}$$

or, in general,

$$\left\langle x\,\middle|\,x'\right\rangle = \left\langle x'\,\middle|\,x\right\rangle = \delta(x-x') \tag{2.391}$$

We then have for each real number a

$$x\delta(x-a) = a\delta(x-a) \tag{2.392}$$

which is a *valid mathematical relation* for delta functions.

Thus, we can formally use Dirac delta functions for eigenfunctions of $\hat{Q}$ as follows: for each real number a we have

$$x\delta(x-a) = a\delta(x-a) \tag{2.393}$$

If we write $|a\rangle$ for $\delta(x-a)$, we then have

$$\hat{Q}\,|a\rangle = a\,|a\rangle \tag{2.394}$$

We must not consider $\delta(x-a)$ as a standard integrable function and we cannot think of $|a\rangle$ as a vector in the Hilbert space L^2. We must do all mathematics using the standard delta function rules.

In this way we have

$$\langle a\,|\,g\rangle = g(a) = \int_{-\infty}^{\infty} \delta(x-a)g(x)\,dx \tag{2.395}$$

as the components of a vector $|g\rangle$ in the spectral representation of $\hat{Q}$.

Note the shift from a function $g(x)$ to the ket vector $|g\rangle$ and the relationship between the two mathematical objects. In fact, we can write

$$\begin{aligned} g(x) &= \int_{-\infty}^{\infty} \delta(x-a)g(a)\,da = \langle x\,|\,g\rangle = \langle x|\,\hat{I}\,|g\rangle \\ &= \langle x|\left(\int_{-\infty}^{\infty} |a\rangle\,\langle a|\;da\right)|g\rangle = \langle x|\int_{-\infty}^{\infty} \langle a\,|\,g\rangle\,|a\rangle\;da \end{aligned} \tag{2.396}$$

or

$$|g\rangle = \int_{-\infty}^{\infty} \langle a\,|\,g\rangle\,|a\rangle\;da \tag{2.397}$$

In addition, we have (using the properties of projection operators derived earlier)

$$\begin{aligned} \langle a\,|\,g\rangle &= \langle a|\,\hat{I}\,|g\rangle = \langle a|\int |x\rangle\,\langle x|\;dx\,|g\rangle \\ &= \int \langle a\,|\,x\rangle\,\langle x\,|\,g\rangle\;dx = \int \delta(x-a)g(x)\,dx \\ &= g(a) \end{aligned} \tag{2.398}$$

as expected.

Thus, formally, we can think of any eigenfunction $g(x)$ as a linear combination of delta functions, where the delta functions are analogous to an orthonormal basis of eigenvectors with the symbol $|x\rangle$. We the have

$$|g\rangle = \int_{-\infty}^{\infty} \langle x \,|\, g\rangle \, |x\rangle \; dx \quad , \quad \hat{I} = \int_{-\infty}^{\infty} |x\rangle \, \langle x| \; dx \tag{2.399}$$

Thus, for each real number a, we define the operator $|a\rangle \, \langle a|$ by

$$(|a\rangle \, \langle a| \, g)(x) = \langle x \,|\, a\rangle \, \langle a \,|\, g\rangle = g(a)\delta(x-a) \tag{2.400}$$

$$|a\rangle \, \langle a| \, g = \langle a \,|\, g\rangle \, |a\rangle = g(a) \, |a\rangle \tag{2.401}$$

In a similar manner, the projection operator $\hat{E}_x$ in the spectral decomposition of $\hat{Q}$ is given by

$$(\hat{E}_x g)(y) = \int_{-\infty}^{x} g(a)\delta(y-a) \, da \tag{2.402}$$

which we can write as

$$(\hat{E}_x g)(y) = \int_{-\infty}^{x} (|a\rangle \langle a| \, g)(y) \, da \tag{2.403}$$

This says that

$$\hat{E}_x = \int_{-\infty}^{x} |a\rangle \langle a| \, da \tag{2.404}$$

Finally, we have

$$\hat{Q} = \int_{-\infty}^{\infty} x \, d\hat{E}_x \tag{2.405}$$

which we write as

$$\hat{Q} = \int_{-\infty}^{\infty} x \, |x\rangle \langle x| \, dx \tag{2.406}$$

This is analogous to a sum of eigenvalues multiplying projection operators onto eigenvector subspaces. We will return to this discussion when we introduce the position operator.

2.21 **Another Continuous Spectrum Operator**

We already have the relation

$$\left\langle x \,\middle|\, x' \right\rangle = \delta(x - x') \tag{2.407}$$

Let us introduce a new operator $\hat{p}$ such that

$$\hat{p}\,|p\rangle = p\,|p\rangle \quad , \quad -\infty \leq p \leq \infty \quad , \quad p \text{ real} \tag{2.408}$$

Thus $\hat{p}$ is an operator with a continuous spectrum just like $\hat{Q}$. As we found to be true for $\hat{Q}$, we can now also write

$$\hat{p} = \frac{1}{2\pi\hbar} \int p\,|p\rangle\,\langle p|\; dp \qquad , \qquad \hat{I} = \frac{1}{2\pi\hbar} \int |p\rangle\,\langle p|\; dp \tag{2.409}$$

This allows us to write

$$\begin{aligned} \left\langle x' \,\middle|\, x \right\rangle = \delta(x' - x) = \left\langle x' \right| \hat{I}\,|x\rangle &= \frac{1}{2\pi\hbar} \int \left\langle x' \right| (|p\rangle\,\langle p|\,|x\rangle\; dp \\ &= \frac{1}{2\pi\hbar} \int \left\langle x' \,\middle|\, p \right\rangle \langle p \,|\, x\rangle\; dp = \frac{1}{2\pi\hbar} \int \left\langle x' \,\middle|\, p \right\rangle \langle x \,|\, p\rangle^*\; dp \end{aligned} \tag{2.410}$$

Now, one of the standard representations of the delta function is

$$\delta(x - x') = \frac{1}{2\pi\hbar} \int e^{-ip(x-x')/\hbar}\, dp \tag{2.411}$$

Thus we can write

$$\int \langle x' \,|\, p\rangle \langle x \,|\, p\rangle^* \; dp = \int e^{-ip(x-x')/\hbar}\, dp \tag{2.412}$$

One of the most important solutions to this equation is

$$\langle x \,|\, p\rangle = e^{ipx/\hbar} \rightarrow \langle x \,|\, p\rangle^* = e^{-ipx/\hbar} \quad , \quad \langle x' \,|\, p\rangle = e^{ipx'/\hbar} \tag{2.413}$$

As we shall see later, this choice will correspond to the new operator $\hat{p}$ representing the standard linear momentum. We can then write

$$\langle x|\, \hat{p}\, |p\rangle = p \langle x \,|\, p\rangle = p e^{ipx/\hbar} = -i\hbar \frac{\partial}{\partial x} e^{ipx/\hbar} = -i\hbar \frac{\partial}{\partial x} \langle x \,|\, p\rangle \tag{2.414}$$

which, in our earlier notation, says

$$(\hat{p}g)(x) = -i\hbar\frac{\partial}{\partial x}g(x) \tag{2.415}$$

In addition we can write

$$\begin{aligned}
&\langle p|\,\hat{x}\,|\psi\rangle = [\langle\psi|\,\hat{x}\,|p\rangle]^* = \left[\langle\psi|\,\hat{x}\left(\int |x'\rangle\langle x'|\;dx'\right)|p\rangle\right]^* \\
&= \left[\int \langle\psi|\,\hat{x}\,|x'\rangle\langle x'\,|\,p\rangle\;dx'\right]^* = \left[\int x'\langle\psi\,|\,x'\rangle\langle x'\,|\,p\rangle\;dx'\right]^* \\
&= \left[\int \langle\psi\,|\,x'\rangle\,x'\langle x'\,|\,p\rangle\;dx'\right]^* = \left[\int \langle\psi\,|\,x'\rangle\left(-i\hbar\frac{\partial}{\partial p}\right)\langle x'\,|\,p\rangle\;dx'\right]^* \\
&= \left[\left(-i\hbar\frac{\partial}{\partial p}\right)\int \langle\psi\,|\,x'\rangle\langle x'\,|\,p\rangle\;dx'\right]^* \\
&= i\hbar\frac{\partial}{\partial p}\left[\langle\psi|\left(\int |x'\rangle\langle x'|\;dx'\right)|p\rangle\right]^* = i\hbar\frac{\partial}{\partial p}\left[\langle\psi\,|\,p\rangle\right]^* = i\hbar\frac{\partial}{\partial p}\langle p\,|\,\psi\rangle \\
&\Rightarrow \langle p|\,\hat{x} = i\hbar\frac{\partial}{\partial p}\langle p|
\end{aligned} \tag{2.416}$$

since $|\psi\rangle$ is arbitrary.

Now, since the eigenvectors of $\hat{p}$ form a basis, we can write any arbitrary vector as

$$|g\rangle = \int \langle p \,|\, g\rangle \, |p\rangle \; dp \tag{2.417}$$

which implies

$$\langle x \,|\, g\rangle = \int \langle p \,|\, g\rangle \, \langle x \,|\, p\rangle \; dp = \int \langle p \,|\, g\rangle \, e^{ipx/\hbar} \, dp \tag{2.418}$$

Now the theory of Fourier transforms says that

$$g(x) = \int G(p) e^{ipx/\hbar} \, dp \tag{2.419}$$

where $G(p)$ is the Fourier transform of $g(x)$. Thus, we find that $G(p) = \langle p \,|\, g\rangle$ is the Fourier transform of $g(x)$.

More about Fourier Transforms (in general)

In the space L^2 of square-integrable functions, let us consider a self-adjoint operator defined by the relation we found earlier for the $\hat{p}$ operator

$$(\hat{p}g)(x) = -i\hbar\frac{\partial}{\partial x}g(x) \tag{2.420}$$

As we already have seen there is a direct connection here to Fourier transforms. Let us review some of the mathematical concepts connected with the *Fourier Transform*.

If g is a function(vector) in L^2, then

$$\psi_n(k) = \frac{1}{2\pi}\int_{-n}^{n} e^{-ikx}g(x)\,dx \tag{2.421}$$

defines a sequence of functions(vectors) ψ_n in L^2 which converges as $n \to \infty$ to a limit function(vector) Gg such that $\|Gg|^2 = \|g\|^2$ and

$$\psi(k) = (Gg)(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}g(x)\,dx \tag{2.422}$$

We also have

$$g_n(k) = \frac{1}{2\pi} \int_{-n}^{n} e^{ikx} (Gg)(k)\, dk \tag{2.423}$$

which defines a sequence of functions(vectors) that converges to g as $n \to \infty$ where

$$g(x) = \frac{1}{2\pi} \int (Gg)(k) e^{ikx}\, dk \tag{2.424}$$

Now, this gives

$$(\hat{p}g)(x) = -i\hbar \frac{\partial}{\partial x} g(x) = \frac{\hbar}{2\pi} \int (Gg)(k) k e^{ikx}\, dk \tag{2.425}$$

It is clear from this expression that a vector g is in the domain of $\hat{p}$ if and only if the quantity $k(Gg)(k)$ is square-integrable. We then have

$$
\begin{aligned}
(G\hat{p}g)(k) &= \frac{1}{2\pi}\int (\hat{p}g)(x)e^{-ikx}\,dx \\
&= \frac{1}{2\pi}\int \frac{1}{2\pi}\left(\int (Gg)(k')\hbar k' e^{ik'x}\,dk'\right)e^{-ikx}\,dx \\
&= \frac{1}{2\pi}\int (Gg)(k')\hbar k'\,dk' \frac{1}{2\pi}\int e^{i(k'-k)x}\,dx \\
&= \frac{1}{2\pi}\int (Gg)(k')\hbar k'\delta(k'-k)\,dk' = k(Gg)(k) \qquad (2.426)
\end{aligned}
$$

We call G the *Fourier transform* of g. G is a unitary operator on L^2 . Its inverse is given by

$$
(G^{-1}h)(x) = \frac{1}{2\pi}\int h(k)e^{ikx}\,dk \qquad (2.427)
$$

which implies

$$
(G^{-1}h)(x) = (Gh)(-x) \qquad (2.428)
$$

for every h.

Since G is unitary, it preserves inner products as well as lengths of vectors so we have

$$\int (Gh)(k)^*(Gg)(k)\,dk = \int h^*(x)g(x)\,dx \tag{2.429}$$

for all vectors h and g.

In terms of the operator $\hat{Q}$ defined by

$$(\hat{Q}g)(x) = xg(x) \tag{2.430}$$

it can be shown that

$$G\hat{p} = \hat{Q}G \tag{2.431}$$

or

$$\hat{p} = G^{-1}\hat{Q}G \tag{2.432}$$

From the spectral decomposition

$$\hat{Q} = \int_{-\infty}^{\infty} y \, d\hat{E}_y \tag{2.433}$$

we can then obtain the spectral decomposition of $\hat{p}$. Since G is unitary and the set of operators $G^{-1}\hat{E}_y G$ is a spectral family of projection operators, the set of operators $\hat{E}_y$ is also a spectral family of projection operators.

Since $G^{-1} = G^{\dagger}$, we have

$$\begin{aligned}(h, \hat{p}g) &= (h, G^{\dagger}\hat{Q}Gg) = (Gh, \hat{Q}Gg) \\ &= \int_{-\infty}^{\infty} y \, d(Gh, \hat{E}_y Gg) = \int_{-\infty}^{\infty} y \, d(h, G^{-1}\hat{E}_y Gg)\end{aligned} \tag{2.434}$$

for any vector h and any vector g in the domain of $\hat{p}$. Thus the spectral decomposition of $\hat{p}$ is

$$\hat{p} = \int_{-\infty}^{\infty} y \, d(G^{-1}\hat{E}_y G) \tag{2.435}$$

Now recall that $\hat{E}_y$ is the projection operator onto the subspace of all vectors g such that $g(x) = 0$ for $x > y$. Therefore, $G^{-1}\hat{E}_y G$ is the projection operator onto the subspace of all vectors g such that $(Gg)(k) = 0$ for $k > y$.

This means that $\hat{p}_r$ has the same spectrum as $\hat{Q}_r$, namely, a purely continuous spectrum consisting of all real numbers as we already assumed at the beginning of our discussion. These results generalize to functions of the operators.

We have been thinking of the Fourier transform as an operator G which takes a vector g to a different vector Gg. We may also think of $g(x)$ and $(Gg)(k)$ as two different ways of representing the same vector g as a function. We can write

$$\langle k \,|\, g \rangle = (Gg)(k) \tag{2.436}$$

provided we are careful not to confuse this with

$$\langle x \,|\, g \rangle = g(x) \tag{2.437}$$

We think of $\langle k \,|\, g \rangle$ as a function on the spectra of $\hat{p}$. We then have

$$\langle k | \, \hat{p} \, | g \rangle = k \, \langle k \,|\, g \rangle \tag{2.438}$$

which is the spectral representation of $\hat{p}$.

For a function f of $\hat{p}$ we have

$$\langle k | \, f(\hat{p}) \, | g \rangle = f(k) \, \langle k \,|\, g \rangle \tag{2.439}$$

The operator $\hat{p}$ has no eigenvectors (as was true earlier for $\hat{Q}$), It does, however, have eigenfunctions which we can use as analogs of eigenvectors as we did earlier for $\hat{Q}$.

If we write $|k\rangle$ for

$$\frac{1}{\sqrt{2\pi}} e^{ikx} \tag{2.440}$$

we have

$$\hat{p}\,|k\rangle = \hbar k\,|k\rangle \tag{2.441}$$

as we assumed at the beginning, since

$$-i\hbar\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{2\pi}}e^{ikx}\right) = \hbar k\left(\frac{1}{\sqrt{2\pi}}e^{ikx}\right) \tag{2.442}$$

For the components of a vector g n the spectral representation of the operators $\hat{p}$ we have

$$\langle k\,|\,g\rangle = (Gg)(k) = \frac{1}{\sqrt{2\pi}}\int g(x)e^{-ikx}\,dx \tag{2.443}$$

We can think of these as the inner products of g with the eigenfunctions $e^{ikx}/\sqrt{2\pi}$. We have also

$$g(x) = \frac{1}{\sqrt{2\pi}}\int (Gg)(k)e^{ikx}\,dk \tag{2.444}$$

which we can write as

$$|k\rangle = \int \langle k \,|\, g\rangle \, |k\rangle \; dk \tag{2.445}$$

so we can think of any vector g as a linear combination of the eigenfunctions.

Thus, the eigenfunctions $e^{ikx}/\sqrt{2\pi}$ are analogous to an orthonormal basis of eigenvectors. They are not vectors in the Hilbert space L^2, however, because they are not square-integrable.

We use them in the same way that we earlier used the delta functions for eigenfunctions of the operators $\hat{Q}$. In fact,

$$\frac{1}{\sqrt{2\pi}} e^{ikx} = \frac{1}{\sqrt{2\pi}} \int \delta(k' - k) e^{ik'x} \, dk' \tag{2.446}$$

is the inverse Fourier transform of the delta function. Now let $|k\rangle \langle k|$ be defined by

$$(|k\rangle \langle k \,|\, g\rangle)(x) = (Gg)k \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{2.447}$$

or

$$|k\rangle \langle k| \, g = \langle k \,|\, g\rangle \, |k\rangle \tag{2.448}$$

Then for the projection operators $G^{-1}\hat{E}_y G$ in the spectral decomposition of $\hat{p}$ we can write

$$(G^{-1}\hat{E}_y G g)(x) = \int_{k\leq y} (Gg)k \frac{1}{\sqrt{2\pi}} e^{ikx}\, dk = \int_{k\leq y} (|k\rangle \langle k \,|\, g\rangle)(x)\, dk \tag{2.449}$$

or

$$G^{-1}\hat{E}_y G = \int_{k\leq y} (|k\rangle \langle k| \; dk \tag{2.450}$$

and for the spectral decomposition of the operators $\hat{p}$ we get

$$\hat{p} = \int \hbar k \, |k\rangle \langle k| \; dk \tag{2.451}$$

which is the same spectral decompositions in terms of eigenvalues and eigenvectors that we saw earlier.

Chapter 3 **Probability**

3.1 **Probability Concepts**

Quantum mechanics will necessarily involve probability in order for us to make the connection with experimental measurements.

We will be interested in understanding the quantity

$$P(A|B) = \text{probability of event } A \text{ given that event } B \text{ is true}$$

In essence, event B sets up the conditions or an environment and then we ask about the (conditional) probability of event A given that those conditions exist. All probabilities are conditional in this sense. The | symbol means *given* so that items to the right of this *conditioning* symbol are taken as being true.

In other words, we set up an experimental apparatus, which is expressed by properties B and do a measurement with that apparatus, which is expressed by properties A.

We generate numbers (measurements) which we use to give a value to the quantity $P(A|B)$.

3.1.1 **Standard Thinking .....**

We start with the standard mathematical formalism based on *axioms*. We define these events:

1. A = occurrence of A
   (denotes that proposition A is true)
2. $\sim A$ = NOT A = nonoccurrence of A
   (denotes that proposition A is false)
3. $A \cap B$ = A AND B = occurrence of both A and B
   (denotes that proposition A AND B is true)
4. $A \cup B$ = A OR B =occurrence of at least A and B
   (denotes that proposition A OR B is true)

and standard Boolean logic as shown below:

Boolean logic uses the basic statements AND, OR, and NOT. Using these and a series of Boolean expressions, the final output would be one TRUE or FALSE statement.

This is illustrated below:

1. If A is true AND B is true, then (A AND B) is true
2. If A is true AND B is false, then (A AND B) is false
3. If A is true OR B is false, then (A OR B) is true
4. If A is false OR B is false, then (A OR B) is false

or written as a *truth table*:

A	B	$(A \cap B)$	$(A \cup B)$
1	1	1	1
1	0	0	1
0	1	0	1
0	0	0	0

Table: Boolean Logic

where 1 = TRUE and 0 = FALSE.

Then we set up a theory of probability with these axioms: 1. $P(A|A) = 1$

This is the probability of the occurrence A given the occurrence of A. This represents a certainty and, thus, the probability must $= 1$. This is clearly an obvious assumption that we must make if our probability ideas are to make any sense at all.

In other words, if I set the experimental apparatus such that the meter reads A, then it reads A with probability $= 1$.

2. $0 \leq P(A|B) \leq P(B|B) = 1$

This just expresses the sensible idea that no probability is greater than the probability of a certainty and it make no sense to have the probability be less than 0.

3. $P(A|B) + P(\sim A|B) = 1$ or $P(\sim A|B) = 1 - P(A|B)$

This just expresses the fact that the probability of something (anything) happening (A or $\sim A$) given B is a certainty ($= 1$), that is, since the set A or $\sim A$ includes everything that can happen, the total probability that one or the other occurs must be the probability of a certainty and be equal to one.

4. $P(A \cap B|C) = P(A|C)P(B|A \cap C)$

This says that the probability that 2 events A, B both occur given that C occurs equals the probability of A given C multiplied by the probability of B given $(A \cap C)$, which makes sense which makes sense if you think of them happening in sequence.

All other probability relationships can be derived from these axioms.

The nonoccurrence of A given that A occurs must have probability $= 0$. This is expressed by

$$P(\sim A|A) = 0 \tag{3.1}$$

This result clearly follows from the axioms since

$$P(A|B) + P(\sim A|B) = 1 \tag{3.2}$$

$$P(A|A) + P(\sim A|A) = 1 \tag{3.3}$$

$$P(\sim A|A) = 1 - P(A|A) = 1 - 1 = 0 \tag{3.4}$$

Example: Let us evaluate $P(X \cap Y|C) + P(X \cap \sim Y|C)$.

We use axiom (4) in the 1^{st} term with and in the 2^{nd} term with to get

$$
\begin{aligned}
P(X \cap Y|C) + P(X \cap \sim Y|C) & \\
&= P(X|C)P(Y|X \cap C) + P(X|C)P(\sim Y|X \cap C) \\
&= P(X|C)[P(Y|X \cap C) + P(\sim Y|X \cap C)] \\
&= P(X|C)[1] = P(X|C) \qquad (3.5)
\end{aligned}
$$

where we have used axiom (3). Thus we have the result

$$P(X \cap Y|C) + P(X \cap \sim Y|C) = P(X|C) \qquad (3.6)$$

Now let us use this result with $X = \sim A, Y = \sim B$. This gives

$$P(\sim A \cap \sim B|C) + P(\sim A \cap \sim\sim B|C) = P(\sim A|C) \qquad (3.7)$$

$$P(\sim A \cap \sim B|C) + P(\sim A \cap B|C) = 1 - P(A|C) \qquad (3.8)$$

$$P(\sim A \cap \sim B|C) = 1 - P(A|C) - P(\sim A \cap B|C) \qquad (3.9)$$

Then use the result again with $X = B, Y = \sim A$. This gives

$$P(B \cap \sim A|C) + P(B \cap A|C) = P(B|C) \tag{3.10}$$

or

$$P(\sim A \cap B|C) = P(B|C) - P(A \cap B|C) \tag{3.11}$$

which gives

$$P(\sim A \cap \sim B|C) = 1 - P(A|C) - P(B|C) + P(A \cap B|C) \tag{3.12}$$

Now

$$P(A \cup B|C) = 1 - P(\sim (A \cup B)|C) = 1 - P((\sim A \cap \sim B)|C) \tag{3.13}$$

since

$$\sim (A \cup B) = (\sim A \cap \sim B) \tag{3.14}$$

i.e., we can construct a *truth table* as shown below, which illustrates the equality directly

A	B	$(\sim (A \cup B))$	$(\sim A \cap \sim B)$
1	1	0	0
1	0	0	0
0	1	0	1
0	0	1	1

Table: Equivalent Expressions

We finally get

$$P(A \cup B) = P(A|C) + P(B|C) - P(A \cap B|C) \tag{3.15}$$

which is a very important and useful result.

If we have $P(A \cap B|C)$=0, then events A and B are said to be *mutually exclusive* given that C is true and the relation then reduces to

$$P(A \cup B) = P(A|C) + P(B|C) \tag{3.16}$$

This is the rule of *addition of probabilities for exclusive events.*

Some other important results are:

$$If\ A \cap B = B \cap A, |; then\ P(A|C)P(B|A \cap C) = P(B|C)P(A|B \cap C) \tag{3.17}$$

$$If\ P(A|C) \neq 0,\ then\ P(B|A \cap C) = P(A|B \cap C)\frac{P(B|C)}{P(A|C)} \tag{3.18}$$

which is *Baye's theorem.* It relates the probability of B given A to the probability of A given B.

When we say that B is *independent* of A, we will mean

$$P(B|A \cap C) = P(B|C) \tag{3.19}$$

or the occurrence of A has *NO influence* on the probability of B given C.

Using axiom (4) we then have the result:

If A and B are independent given C, then

$$P(A \cap B|C) = P(A|C)P(B|C) \tag{3.20}$$

This is called *statistical* or *stochastic* independence. The result generalizes to a set of events $\{A_i,\ i = 1, 2, \ldots, n\}$. All these events are independent if and only if

$$P(A_1 \cap A_2 \cap \cdots \cap A_m|C) = P(A_1|C)P(A_2|C)\ldots P(A_m|C) \tag{3.21}$$

for all $m \leq n$.

Now let us think about these ideas in another way that has fundamental importance in modern approaches to quantum theory. The fundamental result in this view will turn out to be the Bayes formula and its relationship to measurements.

3.1.2 **Bayesian Thinking .....**

Two Different Axioms

1. If we specify how much we believe something is true, then we must have implicitly specified how much we believe it is false.
2. If we first specify how much we believe that proposition Y is true, and then state how much we believe X is true given that Y is true, then we must implicitly have specified how much we believe that both X and Y are true.

We assign *real* numbers to each proposition in a manner so that the larger the numerical value associated with a proposition, the more we believe it.

Only using the rules of *Boolean logic*, ordinary algebra, and the constraint that if there are several different ways of using the same information, then we should always arrive at the same conclusions independent of the particular analysis-path chosen,

it is then found that this consistency could only be guaranteed if the real numbers we had attached to our beliefs in the various propositions could be *mapped* (or transformed) to another set of *real* positive numbers which obeyed the usual rules of probability theory:

$$prob(X|I) + prob(\sim X|I) = 1 \quad \text{(same as axiom (3))} \tag{3.22}$$

$$prob(X \cap Y|I) = prob(X|Y \cap I) \times prob(Y|I) \text{ (same as axiom (4))} \tag{3.23}$$

The first of these equations is called the sum rule and states (as earlier) that the probability that X is true plus the probability that X is false is equal to one.

The second of these equations is called the product rule. It states (as earlier) that the probability that both X and Y are true is equal to the probability that X is true given that Y is true times the probability that Y is true (independent of X).

Note all the probabilities are conditional on proposition(s) or conditioning(s) I, which denotes the relevant background information on hand. It is important to understand that there is no such thing as an absolute probability (one without prior information).

Baye's Theorem and Marginalization

As before, we can use the sum and product rules to derive other results.

First, starting with the product rule we have

$$prob(X \cap Y|I) = prob(X|Y \cap I) \times prob(Y|I) \tag{3.24}$$

We can rewrite this equation with X and Y interchanged

$$prob(Y \cap X|I) = prob(Y|X \cap I) \times prob(X|I) \tag{3.25}$$

Since the probability that both X and Y are true must be logically the same as the probability that both Y and X are true we must also have

$$prob(Y \cap X|I) = prob(X \cap Y|I) \tag{3.26}$$

or

$$prob(X|Y \cap I) \times prob(Y|I) = prob(Y|X \cap I) \times prob(X|I) \tag{3.27}$$

or

$$prob(X|Y \cap I) = \frac{prob(Y|X \cap I) \times prob(X|I)}{prob(Y|I)} \tag{3.28}$$

which is *Bayes theorem* (as derived earlier).

Most standard treatments of probability do not attach much importance to Bayes' rule.

This rule, which relates $prob(A|B \cap C)$ to $prob(B|A \cap C)$, allows us to turn things around with respect to the conditioning symbol, which leads to a reorientation of our thinking about probability.

The fundamental importance of this property to data analysis becomes apparent if we replace A and B by *hypothesis* and *data*:

$$prob(A|B \cap C) \propto prob(B|A \cap C) \times prob(A|C) \tag{3.28}$$

$$\begin{aligned} &prob(hypothesis|data \cap C) \\ &\quad \propto prob(data|hypothesis \cap C) \times prob(hypothesis|C) \end{aligned} \tag{3.29}$$

Note that the equality has been replaced with a proportionality because the term $prob(data|I) = evidence$ has been omitted. The proportionality constant can be found from the normalization requirement that the sum of the probabilities for something happening must equal 1.

The power of Bayes' theorem lies in the fact that it relates the quantity of interest, the probability that the hypothesis is true given the data, to the term that we have a better chance of being able to assign, the probability that we would have obtained the measured data if the hypothesis was true.

The various terms in Bayes' theorem have formal names.

The term $prob(hypothesis|C) = prior$ probability represents our state of knowledge(or ignorance) about the truth of the hypothesis before we have analyzed the current data. This is modified by the experimental measurements through the term $prob(data|hypothesis \cap C) = likelihood$ function. This product gives $prob(hypothesis|data \cap C) = posterior$ probability representing our state of knowledge about the truth of the hypothesis in the light of the data(after measurements).

In some sense, Bayes' theorem encapsulates the process of learning, as we shall see later.

Second, consider the following results from the product rule

$$prob(X \cap Y|I) = prob(Y \cap X|I) = prob(Y|X \cap I) \times prob(X|I) \tag{3.30}$$

$$prob(X \cap \sim Y|I) = prob(\sim Y \cap X|I) = prob(\sim Y|X \cap I) \times prob(X|I) \tag{3.31}$$

Adding these equations we get

$$\begin{aligned} &prob(X \cap Y|I) + prob(X \cap \sim Y|I) \\ &\qquad = (prob(Y|X \cap I) + prob(\sim Y|X \cap I))\, prob(X|I) \end{aligned} \tag{3.32}$$

Since $prob(Y|X \cap I) + prob(\sim Y|X \cap I) = 1$ we have

$$prob(X \cap Y|I) + prob(X \cap \sim Y|I) = prob(X|I) \tag{3.33}$$

which, again, is the same result as earlier.

If, on the other hand, $Y \rightarrow \{Y_k, k = 1, 2, \ldots, M\}$ representing a set of M alternative possibilities, then we generalize the two-state result above as

$$\sum_{k=1}^{M} prob(X \cap Y_k|I) = prob(X|I) \tag{3.34}$$

We can derive this result as follows

$$prob(X \cap Y_1|I) = prob(Y_1 \cap X|I) = prob(Y_1|X \cap I) \times prob(X|I) \tag{3.35}$$

$$prob(X \cap Y_2|I) = prob(Y_2 \cap X|I) = prob(Y_2|X \cap I) \times prob(X|I) \tag{3.36}$$

$$\ldots\ldots\ldots\ldots \tag{3.37}$$

$$prob(X \cap Y_M|I) = prob(Y_M \cap X|I) = prob(Y_M|X \cap I) \times prob(X|I) \tag{3.38}$$

Adding these equations we get

$$\sum_{k=1}^{M} prob(X \cap Y_k|I) = prob(X|I) \left(\sum_{k=1}^{M} prob(Y_k \cap X|I) \right) \quad (3.39)$$

If we assume that the $\{Y_k\}$ form a mutually exclusive and exhaustive set of possibilities, that is, if one of the $Y_k's$ is true, then all the others must be false, we then get

$$\sum_{k=1}^{M} prob(Y_k \cap X|I) = \hat{I} \quad (3.40)$$

which is a normalization condition. This completes the derivation.

If we go to the continuum limit where we consider an arbitrarily large number of propositions about some result (the range in which a given result might lie), then as long as we choose the intervals in a contiguous fashion, and cover a big enough range of values, we will have a mutually exclusive and exhaustive set of possibilities.

In the limit of $M \to \infty$, we obtain

$$prob(X|I) = \int_{-\infty}^{\infty} prob(x \cap Y|I)\, dY \tag{3.41}$$

which is the *marginalization* equation. The integrand here is technically a *probability density function(pdf)* rather than a probability. It is defined by

$$pdf(X \cap Y = y|I) = \lim_{\delta y \to 0} \frac{prob(X \cap y \leq Y \leq y + \delta y|I)}{\delta y} \tag{3.42}$$

and the probability that the value of Y lies in a finite range between y_1 and y_2 (and X is also true) is given by

$$prob(X \cap y_1 \leq Y \leq y_2|I) = \int_{y_1}^{y_2} pdf(X \cap Y|I)\, dY \tag{3.43}$$

which leads directly to the marginalization equation.

In this continuum limit the normalization condition takes the form

$$1 = \int_{-\infty}^{\infty} pdf\,(Y|X \cap I)\,dY \tag{3.44}$$

Marginalization is a very powerful device in data analysis because it enables us to deal with *nuisance parameters*, that is, quantities which necessarily enter the analysis but are of no intrinsic interest. The unwanted background signal present in many experimental measurements, and instrumental parameters which are difficult to calibrate, are examples of nuisance parameters. 3.2 **Probability Interpretation**

In the standard way of thinking about probability in relation to experiments, measured results are related to probabilities using the concept of a *limit frequency*. The limit frequency is linked to probability by this definition:

> If C can lead to either A or $\sim A$ and if in n repetitions, A occurs m times, then

$$P(A|C) = \lim_{n\to\infty} \frac{m}{n} \tag{3.45}$$

We must now connect the mathematical formalism with this limit frequency concept so that we can use the formalism to make predictions for experiments in real physical systems.

This approach depends on whether we can prove that the limit makes sense for real physical systems. Let us see how we can understand the real meaning of the above interpretation of probability and thus learn how to use it in quantum mechanics, where probability will be the dominant property.

Suppose that we have an experimental measurement, M, that can yield either A or $\sim A$ as results, with a probability for result A given by

$$P(A|M) = p \tag{3.46}$$

In general, we let any sequence of n independent measurements be labeled as event M^n and we define n_A as the number of times A occurs, where $0 \leq n_A \leq n$.

Now imagine we carry out a sequence of n independent measurements and we find that A occurs r times. The probability for a sequence of results that includes result A occurring r times and $\sim A$ occurring $(n-r)$ times (independent of their order in the sequence) is given by

$$p^r q^{n-r} \tag{3.47}$$

where

$$q = P(\sim A|M) = 1 - P(A|M) = 1 - p \tag{3.48}$$

The different sequence orderings are mutually exclusive events and thus we have

$$P(n_A = r|M^n) = \sum_{all\ possible\ orderings} p^r q^{n-r} \tag{3.49}$$

The sum

$$\sum_{all\ possible\ orderings} \tag{3.50}$$

just counts the number of ways to distribute r occurances of A and (n-r) occurances of $\sim A$, where all the terms contain the common factor $p^r q^{n-r}$. This result is given by the Binomial probability distribution (more about this later) as

$$\frac{n!}{r!(n-r)!} \tag{3.51}$$

so that

$$P(n_A = r|M^n) = \frac{n!}{r!(n-r)!} p^r q^{n-r} \tag{3.52}$$

Now to get to the heart of the problem.

The frequency of A in M^n is given by

$$f_n = \frac{n_A}{n} \tag{3.53}$$

This is *not necessarily* $= p$ in any set of measurements.

What is the relationship between them? Consider the following:

$$\begin{aligned}
\langle n_A \rangle &= \text{ average or expectation value} \\
&= \text{ sum over [possible values times probability of that value} \\
&= \sum_{r=0}^{n} r P(n_A = r | M^n) = \sum_{r=0}^{n} r \frac{n!}{r!(n-r)!} p^r q^{n-r}
\end{aligned} \tag{3.54}$$

We now use a clever mathematical trick to evaluate this sum. For the moment consider p and q to be two arbitrary independent variables. At the end of the calculation we will let $q = 1 - p$ as is appropriate for a real physical system.

From the Binomial expansion formula, we have, in general,

$$\sum_{r=0}^{n} \frac{n!}{r!(n-r)!} p^r q^{n-r} = (p+q)^n \tag{3.55}$$

We then have

$$p\frac{\partial}{\partial p} \sum_{r=0}^{n} \frac{n!}{r!(n-r)!} p^r q^{n-r} = p\frac{\partial}{\partial p}(p+q)^n \tag{3.56}$$

so that

$$\sum_{r=0}^{n} r\frac{n!}{r!(n-r)!} p^r q^{n-r} = np(p+q)^{n-1} \tag{3.57}$$

This gives

$$\sum_{r=0}^{n} rP(n_A = r|M^n) = np(p+q)^{n-1} \tag{3.58}$$

or

$$\langle n_A \rangle = np(p+q)^{n-1} \tag{3.59}$$

In a real physical system, we must have $p + q = 1$, so that we end up with the result

$$\langle n_A \rangle) = np \tag{3.60}$$

and

$$\langle f_n \rangle = \frac{\langle n_A \rangle}{n} = p \tag{3.61}$$

This says that $p =$ the average frequency.

This does not say, however, that f_n is close to p.

Now consider a more general experiment where the outcome of a measurement is the value of some continuous variable Q, with probability density (for its continuous spectrum) given by

$$P(q < Q < q + dq|M) = h(q)dq \tag{3.62}$$

If we let $h(q)$ contain delta-functions, then this derivation is also valid for the discrete part of the spectrum. We can now derive the following useful result. If Q is a nonnegative variable, which means that $h(q) = 0$ for $q < 0$, then for any $\epsilon > 0$

$$\langle Q \rangle = \int_0^\infty h(q) q \, dq \geq \int_\epsilon^\infty h(q) q \, dq \geq \epsilon \int_\epsilon^\infty h(q) \, dq = \epsilon P(Q \geq \epsilon|M) \tag{3.63}$$

This implies that

$$P(Q \geq \epsilon|M) \leq \frac{\langle Q \rangle}{\epsilon} \tag{3.64}$$

Now we apply this result to the nonnegative variable $|Q - c|^\alpha$ where $\alpha > 0$ and $c =$ number, to obtain

$$P(|Q-c| \geq \epsilon|M) = P(|Q-c|^\alpha \geq \epsilon^\alpha|M) \leq \frac{\langle|Q-c|^\alpha\rangle}{\epsilon^\alpha} \quad (3.65)$$

which is called *Chebyshev's inequality.*

In the special case where $\alpha = 2, c = \langle Q\rangle$=mean of distribution we have

$$\langle|Q-c|^2\rangle = \langle|Q-\langle Q\rangle|^2\rangle = -\langle Q^2\rangle - \langle Q^2\rangle^2 = \sigma^2 = \text{ variance} \quad (3.66)$$

so that letting $\epsilon = k\sigma$ we get

$$P(|Q-\langle Q\rangle| \geq k\sigma|M) \leq \frac{1}{k^2} \quad (3.67)$$

or, the probability of Q being k or more standard deviations from the mean is no greater than $1/k^2$ (*independent* of the form of the probability distribution).

In a similar manner, it can also be shown that

$$P(|f_n - p| \geq \delta | M) \leq \frac{1}{n\delta^2} \tag{3.68}$$

which implies that the probability of f_n (the relative frequency of A in n independent repetitions of M) being more than δ away from p converges to 0 as $n \to \infty$. This is an example of the *law of large numbers* in action. This *DOES NOT* say $f_n = p$ at any time or that f_n remains close to p as $n \to \infty$.

It DOES say that the deviation of f_n from p becomes more and more improbable or that the probability of any deviation approaches 0 as $n \to \infty$.

It is in this sense that one uses the limit frequency from experiment to compare with theoretical probability predictions in physics. *From probability theory one derives only statements of probability, not of necessity.*

3.3 First hints of "subversive" or "Bayesian" thinking.....

How do we reason in situations where it is not possible to argue with certainty? In other words, is there a way to use the techniques of deductive logic to study the inference problem arising when using inductive logic? *No matter what scientists say, this is what they are actually doing most of the time.*

The answer to this last question resides in the Bayes' rule.

To Bayes(along with Bernoulli and Laplace), a probability represented a "degree-of-belief" or "plausibility", that is, how much one thinks that something is true, *based* on the *evidence on hand.*

The developers of standard probability theory(Fisher, Neyman and Pearson) thought this seemed too vague and subjective a set of ideas to be the basis of a "rigorous" mathematical theory.

Therefore, they *defined* probability as the long-run relative frequency with which an event occurred, given *infinitely many repeated* experimental trials. Since such probabilities can be measured, probability was then thought to be an objective tool for dealing with random phenomena.

This frequency definition certainly *seems* to be more objective, but it turns out that its *range of validity* is far more limited.

In this Bayesian view, probability represents a *state of knowledge*. The conditional probabilities represent *logical* connections rather than *causal* ones.

Example:

Consider an urn that contains 5 red balls and 7 green balls.

If a ball is selected at *random*, then we would all agree that the probability of picking a red ball would be 5/12 and of picking a green ball would be 7/12.

If the ball is not returned to the urn, then it seems reasonable that the probability of picking a red or green ball must depend on the outcome of the first pick (because there will be one less red or green ball in the urn).

Now suppose that we are not told the outcome of the first pick, but are given the result of the second pick. Does the probability of the first pick being red or green change with the knowledge of the second pick?

Initially, many observers would probably say *no*, that is, at the time of the first draw, there were still 5 red balls and 7 green balls in the urn, so the probabilities for picking red and green should still be 5/12 and 7/12 independent of the outcome of the second pick. The error in this argument becomes clear if we consider the extreme example of an urn containing only 1 red and 1 green ball.

Although, the second pick cannot affect the first pick in a physical sense, a knowledge of the second result does influence what we can infer about the outcome of the first pick, that is, if the second ball was green, then the first ball must have been red, and vice versa.

We can calculate the result as shown below:

Y = pick is GREEN (2^{nd} pick)

X = pick is RED (1^{st} pick)

I = initial number of RED/GREEN balls = (n, m)

A Bayesian would say:

$$prob(X|Y \cap I) = \frac{prob(Y|X \cap I) \times prob(X|I)}{prob(Y|I)} \tag{3.69}$$

$$prob(X|Y \cap \{n,m\}) = \frac{prob(Y|X \cap \{n,m\}) \times \frac{n}{n+m}}{\frac{n}{n+m}\frac{m}{n+m-1} + \frac{m}{n+m}\frac{m-1}{n+m-1}}$$
$$= \frac{\frac{m}{n+m-1} \times n}{\frac{nm}{n+m-1} + \frac{m(m-1)}{n+m-1}} = \frac{n}{n+m-1} \quad (3.70)$$

$$n = m = 1 \Rightarrow prob(X|Y \cap \{1,1\}) = \frac{1}{1+1-1} = 1 \quad (3.71)$$

$$n = 5, m = 7 \Rightarrow prob(X|Y \cap \{5,7\}) = \frac{5}{5+7-1} = \frac{5}{11} = 0.456 \quad (3.72)$$

Non-Bayesian says:

$$prob(X|\{5,7\}) = \frac{5}{12} = 0.417 \quad (3.73)$$

Clearly, the Bayesian and Non-Bayesian disagree.

However, the non-Bayesian is just *assuming* that the calculated result 0.417 is correct, whereas, the Bayesian is using the rules of probability (Bayes' Rule) to infer the result 0.456 *correctly*.

The concerns about the subjectivity of the Bayesian view of probability are understandable. I think that the presumed shortcomings of the Bayesian approach merely reflect a confusion between subjectivity and the difficult technical question of how probabilities(especially prior probabilities) should be assigned.

The popular argument is that if a probability represents a degree-of-belief, then it must be subjective, because my belief could be different from yours. The Bayesian view is that a probability does indeed represent how much we believe that something is true, but that this belief should be based on all the relevant information available(all prior probabilities).

While this makes the assignment of probabilities an open-ended question, because the information available to me may not be the same as that available to you, it is not the same as subjectivity. It simply means that probabilities are *always conditional*, and this conditioning must be stated *explicitly*.

Objectivity demands only that two people having the same information should assign the same probability.

Cox looked at the question of plausible reasoning from the perspective of logical consistency. He found that the only rules that worked were those of probability theory! Although the sum and product rules of probability are straightforward to prove for frequencies (using Venn diagrams), Cox showed that their range of validity goes much further. Rather than being restricted to frequencies, he showed that probability theory constitutes the basic calculus for logical and consistent plausible reasoning, which means scientific inference!

Another Example - Is this a fair coin?

We consider a simple coin-tossing experiment. Suppose that I had found this coin and we observed 4 heads in 11 flips.

If by the word *fair* we mean that we would be prepared to make a $50:50$ bet on the outcome of a flip being a head or a tail, then do you think that it is a fair coin?

If we ascribe fairness to the coin, then we naturally ask how sure are we that this was so or if it was not fair, how unfair do we think it was?

A way of formulating this problem is to consider a large number of *contiguous* hypotheses about the range in which the *bias-weighting* of the coin might lie. If we denote bias-weighting by H, then $H = 0$ and $H = 1$ can represent a coin which produces a tail(not a head!) or a head on every flip, respectively.

There is a continuum of possibilities for the value of H between these limits, with $H = 1/2$ indicating a fair coin. The hypotheses might then be, for example

$$\text{(a) } 0.00 \leq H \leq 0.01$$
$$\text{(b) } 0.01 \leq H \leq 0.03$$
$$\text{(c) } 0.02 \leq H \leq 0.03$$
$$\text{and so on}$$

Our state of knowledge about the fairness, or the degree of unfairness, of the coin is then completely summarized by specifying how much we believe these various hypotheses to be true. If we assign a high probability to one (or a closely grouped few) of these hypotheses, compared to others, then this indicates that we are confident in our estimate of the bias-weighting.

If there was no such distinction, then it would reflect a high level of ignorance about the nature of the coin.

In this case, our inference about the fairness of the data is summarized by the conditional pdf $prob(H|\{data\}H \cap I)$. This is just a representation of the limiting case of a continuum of hypotheses for the value of H, that is, the probability that H lies in an infinitesimally narrow range between h and $h + \delta h$ is given by $prob(H = h|\{data\} \cap I)\, dH$. To estimate this posterior pdf, we need to use Baye's theorem, which relates the pdf of interest to two others that are easier to assign:

$$prob(H|\{data\} \cap I) \propto prob(\{data\}|H \cap I) \times prob(H|I) \quad (3.74)$$

We have omitted the denominator $prob(\{data\}|I)$ since it does not involve bias-weighting explicitly and replaced the equality by a proportionality. The omitted constant can be determined by normalization

$$\int_0^1 prob(H|\{data\} \cap I)\, dH = 1 \quad (3.75)$$

The prior pdf, $prob(H|I)$, on the right side represents what we know about the coin given only that I found the coin. This means that we should keep an open mind about the nature of the coin. A simple probability assignment which reflects this is a uniform pdf

$$prob(H|I) = \begin{cases} 1 & 0 \leq H \leq 1 \\ 0 & \text{otherwise} \end{cases} \tag{3.76}$$

This prior state of knowledge (or ignorance) is modified by the data through the likelihood function, $prob(\{data\}|H \cap I)$, which is a measure of the chance that we would have obtained the data we actually observed if the value of the bias-weighting H was given (as known). If, in the conditioning information I, we assume that the flips of the coin were independent events, so that the outcome of one did not influence that of another, then the probability of obtaining the data R heads in N tosses is given by the binomial distribution

$$prob(\{data\}|H \cap I) \propto H^R(1-H)^{N-R} \tag{3.77}$$

The product of these last two results then gives the posterior pdf that we require.

It represents our state of knowledge about the nature of the coin in light of the data.

It is instructive to see how this pdf evolves as we obtain more and more data pertaining to the coin. A computer simulation is shown below allows us to demonstrate what happens in some typical cases.

The simulation allows for three distinct and very different prior probabilities:

(1) Uniform distribution

(2) Gaussian distribution centered around 0.5 with some spread

(3) Sum of two Gaussians with different centers

These prior probabilities represent very different initial knowledge:

(1) total ignorance-we have no idea if it is fair

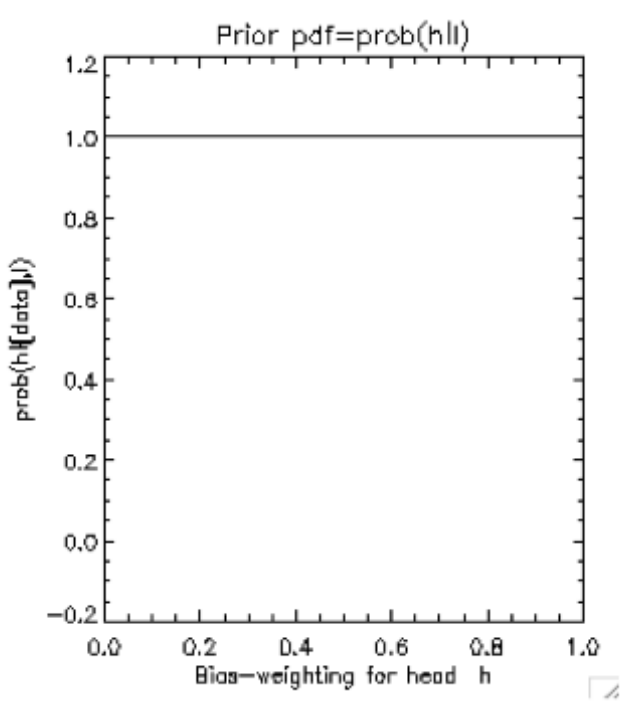
(2) knowledge that mean is 0.5[with spread]-we think it is fair

(3) knowledge that it is unfair (either all tails or all heads) [with spreads]

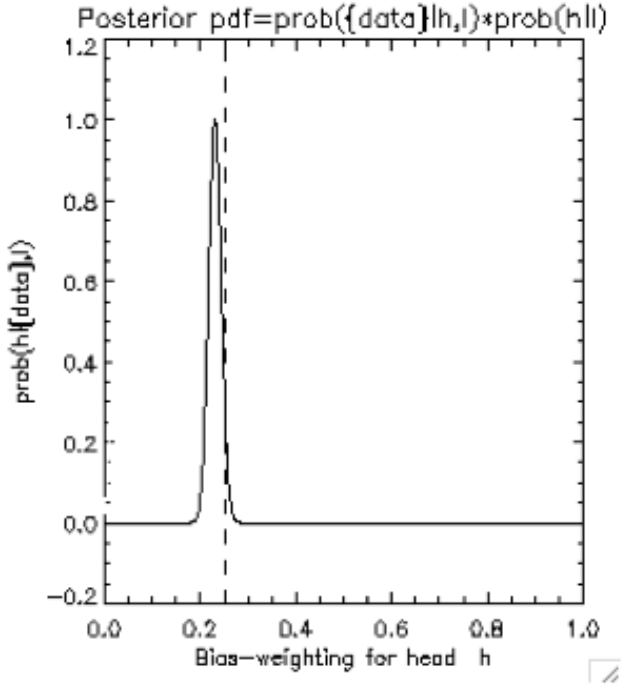
In the simulation we can choose the true mean value (h_0), which is then reflected in the simulated coin tosses (the data).

As can be seen from the images below, the only effect that different prior probabilities have is to change the period of time evolution to the final posterior pdf (which is the same eventually in all cases)!

(1) total ignorance - we have no idea if it is fair



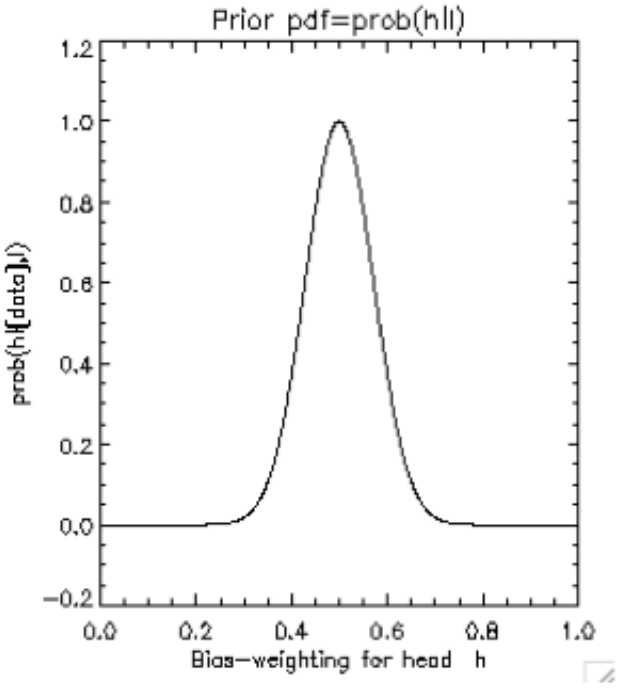
(a) Prior



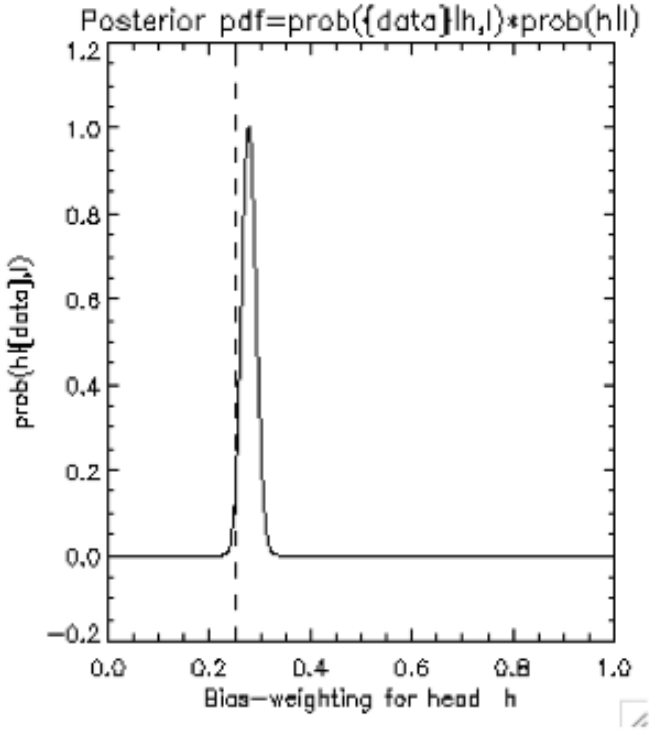
(b) Posterior

Figure: Total Ignorance

(2) knowledge that mean is 0.5 [with spread] - we think it is fair



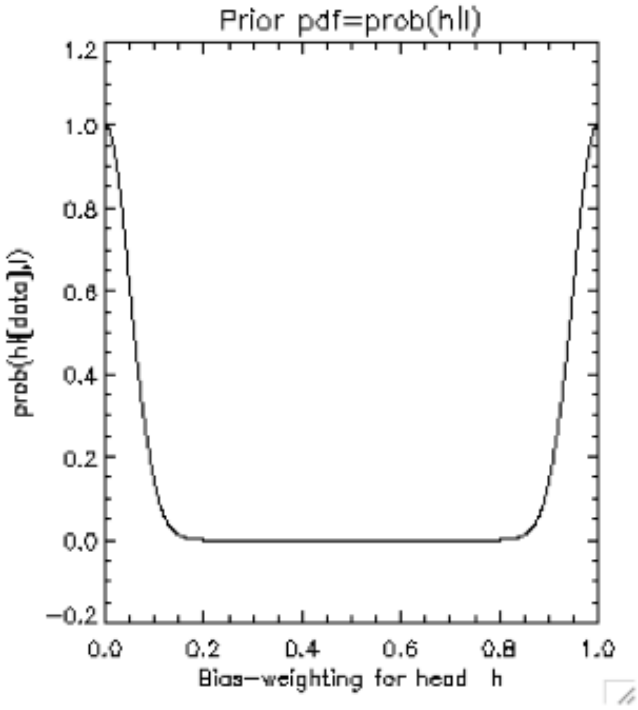
(a) Prior



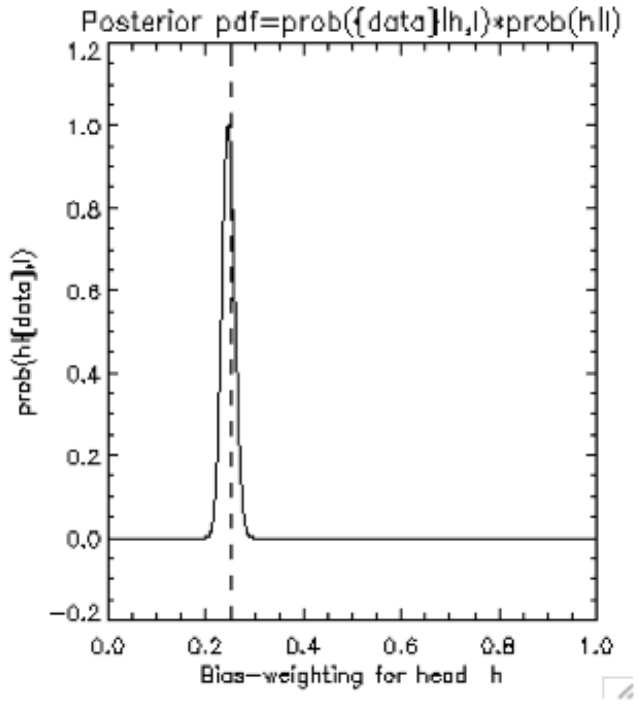
(b) Posterior

Figure: Knowledge that Mean is 0.5

(3) knowledge that it is unfair (either all tails or all heads) [with spreads]



(a) Prior



(b) Posterior

Figure: Knowledge that it is Unfair

In each case, the first figure shows the posterior pdf for H given no data (it is the same as the prior pdf) and the second figure shows the posterior pdf after 1000 tosses and they clearly indicate that no matter what our initial knowledge, the final posterior pdf will be the same, that is, the posterior pdf is dominated by the likelihood function(the actual data) and is independent of the prior pdf.

3.3.1 **The Problem of Prior Probabilities**

We are now faced with the most difficult question. How do we assign probabilities based on prior information?

The oldest idea was devised by Bernoulli - the *principle of insufficient reason* or the *principle of indifference*. It states that if we determine a set of basic, mutually exclusive, possibilities, and we have no reason to believe that any one of them is more likely to be true than another, then we must assign the same *probability* to each of them.

Clearly, this makes sense. Think of flipping a coin with two possibilities, heads and tails. If it is a legitimate coin, then we have no reason to favor heads over tails and we must assign equal probability to each possibility, that is,

$$prob(heads|I) = prob(tails|I) = \frac{1}{2} \tag{3.78}$$

Let us elaborate on the idea of *not having any reason to believe*..... Suppose we had ten possibilities labeled by $X_i, i = 1, 2, \ldots, 10$ and we had no reason to think any was more likely than any other. We would then have

$$prob(X_1|I) = prob(X_2|I) = \ldots = prob(X_{10}|I) = \frac{1}{10} \tag{3.79}$$

Suppose that we relabel or reorder the possibilities. If the conditioning on I truly represents gross ignorance about any details of the situation, then such a reordering should not make any difference in the probability assignments.

Any other statement has to mean that we have other important information besides the simple ordering of the possibilities. For example, imagine that you called a certain side of the coin heads and therefore the other side tails. Nothing changes if your friend switches the meaning of heads and tails. This justification of the Bernoulli principle led Jaynes to suggest that we think of it as a consequence of the *requirement of consistency*.

This principle of insufficient reason can only be applied to a limited set of problems involving games of chance. It leads, however, to some very familiar and very important results if combined with the product and sum rules of probability theory.

Example 1: Assume W white balls and R red balls in an urn. We now pick the balls out of the urn randomly.

The principle of indifference says that we should assign a uniform prior probability (actually a pdf)

$$prob(j|I) = \frac{1}{R+W} \quad , \quad j = 1, 2, 3, \ldots, R+W \tag{3.80}$$

for the proposition that any particular ball, denoted by index j, will be picked. Using the marginalization idea from earlier

$$prob(X|I) = \int_{-\infty}^{\infty} prob(X \cap Y|I)\, dY \tag{3.81}$$

we have

$$\begin{aligned} prob(red|I) &= \sum_{j=1}^{R+W} prob(red \cap j|I) \\ &= \sum_{j=1}^{R+W} prob(j|I) prob(red|j \cap I) \\ &= \frac{1}{R+W} \sum_{j=1}^{R+W} prob(red|j \cap I) \end{aligned} \tag{3.82}$$

where we have used the product rule. The term $prob(red|j \cap I)$ is one if the j^{th} ball is red and zero if it is white. Therefore the summation equals the number of red balls R and we get

$$prob(red|I) = \frac{1}{R+W} \sum_{j=1}^{R+W} prob(red|j \cap I) = \frac{R}{R+W} \qquad (3.83)$$

as expected. However, we have derived this result from the principle of indifference and the product rule. It also follows from the basic notion of probability, that is,

$$prob(red|I) = \frac{\text{number of cases favorable to red}}{\text{total number of equally possible cases}} = \frac{R}{R+W} \qquad (3.84)$$

We now assume that after each pick the ball is returned to the urn and we ask the question: what is the probability that N such picks (trials) will result in r red balls?

Using marginalization and the product rule we can write

$$prob(r|N \cap I) = \sum_k prob(r \cap S_k|N \cap I)$$
$$= \sum_k prob(r|S_k \cap N \cap I) prob(S_k|N \cap I) \quad (3.85)$$

where the summation is over the 2^N possible sequences of red-white outcomes $\{S_k\}$ of N picks. The term $prob(r|S_k \cap N \cap I)$ equals one if S_k contains exactly r red balls and is zero otherwise, so that we need only consider those sequences which have exactly r red outcomes for $prob(S_k|N \cap I)$.

Now we have

$$prob(S_k|N \cap I) = [prob(red|I)]^r \, [prob(white|I)]^{N-r}$$
$$= \frac{R^r W^{N-r}}{(R+W)^N} \quad (3.86)$$

Hence,

$$prob(r|N \cap I) = \frac{R^r W^{N-r}}{(R+W)^N} \sum_k prob(r|S_k \cap N \cap I) \qquad (3.87)$$

for those S_k that matter, i.e., we are only considering those S_k which contain exactly r red balls. In this case we have

$$prob(r|N \cap I) = \frac{R^r W^{N-r}}{(R+W)^N} \frac{N!}{r!(N-r)!} \qquad (3.88)$$

where the last factor just corresponds to the number of sequences (permutations) containing r red balls. Thus,

$$prob(r|N \cap I) = \frac{N!}{r!(N-r)!} p^r (1-p)^{N-r} \qquad (3.89)$$

where

$$p = \frac{R}{R+W} = \text{probability of picking a red ball} \qquad (3.90)$$

and

$$q = 1 - p = \frac{W}{R+W} = \text{probability of picking a white ball} \quad (3.91)$$

Note that $p + q = 1$ as it should since red and white balls are the only possibilities.

We can then compute the frequency r/N with which we expect to observe red balls. We have

$$\begin{aligned}
\langle \frac{r}{N} \rangle &= \sum_{r=0}^{N} \frac{r}{N} prob(r|N \cap I) = \sum_{r=0}^{N} \frac{r}{N} \frac{N!}{r!(N-r)!} p^r (1-p)^{N-r} \\
&= \sum_{r=1}^{N} \frac{(N-1)!}{(r-1)!(N-r)!} p^r (1-p)^{N-r} \\
&= p \sum_{j=0}^{N-1} \frac{(N-1)!}{j!(N-r)!} p^j (1-p)^{N-1-j} \\
&= p(p+q)^{N-1} = p = \frac{R}{R+W} \qquad (3.92)
\end{aligned}$$

as the *expected* or *anticipated* result.

Thus, the expected frequency of red balls, in repetitions of the urn experiment, is equal to the probability of picking one red ball in a single trial. A similar calculation for the mean-square deviation gives the result

$$\langle\Big(\frac{r}{N}-\langle\frac{r}{N}\rangle\Big)^2\rangle=\langle\Big(\frac{r}{N}-p\Big)^2\rangle=\frac{pq}{N} \tag{3.93}$$

Since this becomes zero in the limit of large N, it agrees with the result we derived earlier. It also verifies that Bernoulli's famous theorem or law of large numbers is valid:

$$\lim_{N\to\infty}\left(\frac{r}{N}\right)=prob(red|I) \tag{3.94}$$

This relationship, which allows prediction of the long-run frequency of occurrence from the probability assignment, goes in a direction opposite to the one we want, that is, we would like to be able to determine the probability of obtaining a red ball, in a single pick, given a finite number of observed outcomes. This is, in fact, exactly what Bayes theorem allows us to do!

How do we generalize Bernoulli's principle of insufficient reason to the case of continuous parameters, that is, when the quantity of interest is not restricted to certain discrete values (heads/tails)?

Suppose we have a variable X which represents the position of some object. We then define a probability as follows. Given the information I, the probability that X lies in the infinitesimal range between x and $x + dx$ is

$$prob(X = x|I) = \lim_{\delta x \to 0} prob(x \leq X \leq x + \delta x|I) \qquad (3.95)$$

so that we are treating continuous pdfs as the limiting case of discrete ones. Although it is still awkward to enumerate the possibilities in this case, we can still make use of the principle of consistency which underlies the principle of indifference.

Examples:

A Location Parameter

Suppose that we are unsure about the actual location of the origin. Should this make any difference to the pdf assigned for X? Since I represents gross ignorance about any details of the situation other than the knowledge that X pertains to a location, the answer must be no; otherwise we must already have information regarding the position of the object. Consistency then demands that the pdf for X should not change with the location of the origin or any offset in the position values. Mathematically, we say

$$prob(X|I)\,dX = prob(X + x_0|I)\,d(X + x_0) \tag{3.96}$$

Since x_0 is a constant, $d(X + x_0) = dX$ so that we have

$$prob(X|I) = prob(X + x_0|I) = \text{constant} \tag{3.97}$$

so that the complete ignorance about a location parameter is represented by the assignment of a *uniform* pdf.

A Scale Parameter

Suppose that we have another parameter that tells us about size or magnitude, a so-called *scale* parameter. If we are interested in the size L of some object and we have no idea about the length scale involved, then the pdf should be invariant with respect to shrinking or stretching the length scale. Mathematically, the requirement of consistency can be written

$$prob(L|I)\,dL = prob(\beta L|I)\,d(\beta L) \tag{3.98}$$

where β is a positive constant. Then since $d(\beta L) = \beta\,dL$ we must have

$$prob(L|I) = \beta prob(\beta L|I) \tag{3.99}$$

which can only be satisfied if

$$prob(L|I) \propto \frac{1}{L} \tag{3.100}$$

which is called *Jeffrey's prior*. It represents complete ignorance about the value of a scale parameter.

Now we must have

$$prob(L|I)\, dL = prob(f(L)|I)\, df(L) \tag{3.101}$$

since we are looking at the same domain of values in each case. We then have

$$prob(\log L||)\, d(\log L) = prob(L|I)\, dL \tag{3.102}$$

$$prob(\log L||)\, \frac{dL}{L} = prob(L|I)\, dL \tag{3.103}$$

$$prob(\log L||) = Lprob(L|I) = \text{constant} \tag{3.104}$$

So that assignment of a *uniform* pdf for $\log L$ is the way to represent complete ignorance about a scale parameter.

3.4 **Testable Information: The Principle of Maximum Entropy**

Clearly, some pdfs can be assigned given only the nature of the quantities involved (as we saw above). The methods employed hinge on the use of consistency arguments along with *transformation groups*, which characterize the ignorance for a given situation.

For a set of discrete probabilities(finite) the associated pdf must be invariant with respect to any permutation of the propositions (permutation group). In the continuous parameter case, the associated transformations are translation (origin shift) and dilation (shrink/stretch), which are also group transformations.

Let us move on to a situation where we do not have total ignorance.

Suppose that a die, with the usual six faces, was rolled a very large number of times and we are only told that the average result was 4.5. What probability should we assign for the various outcomes $\{X_i\}$ that the face on top had i dots?

The information or condition I provided by the experiment is written as a simple *constraint* equation

$$\sum_{i=1}^{n} iprob(X_i|I) = 4.5 \tag{3.105}$$

If we had assumed a uniform pdf, then we would have predicted a different average

$$\sum_{i=1}^{n} iprob(X_i|I) = \frac{1}{6}\sum_{i=1}^{n} i = 3.5 \tag{3.106}$$

which means the uniform pdf is not a valid assignment.

There are many pdfs that are consistent with the experimental results. Which one is the best?

The constraint equation above is called *testable information.*

With such a condition, we can either accept or reject any proposed pdf. Jaynes(one of the most brilliant theoretical physicists) proposed that, in this situation, we should make the assignment by using the principle of maximum entropy (**MaxEnt**), that is, we should choose that pdf which has the most entropy S while satisfying the available constraints.

Explicitly, for case in the die experiment above, we need to maximize

$$S = -\sum_{i=1}^{6} p_i \log_e(p_i) \tag{3.107}$$

where $p_i = prob(X_i|I)$ subject to the conditions:

(1) **normalization constraint**

$$\sum_{i=1}^{6} p_i = 1 \tag{3.108}$$

and

(2) **testable information constraint**

$$\sum_{i=1}^{6} i p_i = 4.5 \tag{3.109}$$

Such a constrained optimization is done using the method of *Lagrange multipliers* as shown below.

Define the functions

$$f(p_i) = \sum_{i=1}^{6} p_i - 1 = 0 \Rightarrow \frac{\partial f}{\partial p_j} \equiv 1 \tag{3.110}$$

$$g(p_i) = \sum_{i=1}^{6} ip_i - 4.5 = 0 \Rightarrow \frac{\partial g}{\partial p_j} \equiv j \tag{3.111}$$

The maximization problem can then be written in the following way. Instead we maximize the quantity

$$S + \lambda_f f + \lambda_g g = S \text{ (by definition)} \tag{3.112}$$

where the *constants* are called undetermined or Lagrange multipliers. Thus the maximization equation becomes

$$\frac{\partial S}{\partial p_j} + \lambda_f \frac{\partial f}{\partial p_j} + \lambda_g \frac{\partial g}{\partial p_j} = 0 \quad j = 1, 2, 3, 4, 5, 6 \tag{3.113}$$

We get the equations

$$-\log_e(p_j) - 1 + \lambda_f + j\lambda_g = 0 \quad j = 1, 2, 3, 4, 5, 6 \tag{3.114}$$

and we obtain

$$-\log_e(p_{j+1})-1+\lambda_f+(j+1)\lambda_g = -\log_e(p_j)-1+\lambda_f+j\lambda_g \quad (3.115)$$

This implies that

$$\log_e \frac{p_{j+1}}{p_j} = \lambda_g \Rightarrow \frac{p_{j+1}}{p_j} = \beta = \text{constant} \quad (3.116)$$

This gives

$$-\log_e(p_1) - 1 + \lambda_f + j\log\beta = 0 \Rightarrow \lambda_f = 1 + \log_e \frac{p_1}{\beta} \quad (3.117)$$

Therefore

$$\sum_{i=1}^{6} p_i = 1 = p_1(1 + \beta + \beta^2 + \beta^3 + \beta^4 + \beta^5) \quad (3.118)$$

$$\sum_{i=1}^{6} ip_i = 4.5 = p_1(1 + 2\beta + 3\beta^2 + 4\beta^3 + 5\beta^4 + 6\beta^5) \quad (3.119)$$

or dividing to get rid of p_1 we have

$$\frac{1+2\beta+3\beta^2+4\beta^3+5\beta^4+6\beta^5}{1+\beta+\beta^2+\beta^3+\beta^4+\beta^5}=4.5 \tag{3.120}$$

which gives

$$1.5\beta^5+0.5\beta^4-0.5\beta^3-1.5\beta^2-2.5\beta-3.5=0 \tag{3.121}$$

Solving numerically for β we get 1.449255 so that

$$\begin{aligned}
p_1 &= \frac{1}{1+\beta+\beta^2+\beta^3+\beta^4+\beta^5}=0.05435\\
p_2 &= \beta p_1 = 0.07877\\
p_3 &= \beta p_2 = 0.11416\\
p_4 &= \beta p_3 = 0.16545\\
p_5 &= \beta p_4 = 0.23977\\
p_6 &= \beta p_5 = 0.34749
\end{aligned} \tag{3.122}$$

is the MaxEnt assignment for the pdf for the outcomes of the die roll, given only that it has the usual six faces and yields an average result of 4.5.

Why should the entropy function

$$S = -\sum_{i=1}^{6} p_i \log_e(p_i) \tag{3.123}$$

specified above be the choice for a selection criterion?

Let us look at two examples that suggest this criterion is highly desirable and probably correct.

Kangaroo Problem(Gull and Skilling)

The kangaroo problem is as follows:

Information: 1/3 of all kangaroos have blue eyes and 1/3 of all kangaroos are left-handed

Question: On the basis of this information alone, what proportion of kangaroos are both blue-eyed and left-handed?

For any particular kangaroo, there are four distinct possibilities, namely, that it is

(1) blue-eyed and left-handed

(2) blue-eyed and right-handed

(3) not blue-eyed but left-handed

(4) not blue-eyed but right-handed

Bernoulli's law of large numbers says that the expected values of the fraction of kangeroos with characteristics (1)-(4) will be equal to the probabilities (p_1, p_2, p_3, p_4) we assign to each of these propositions.

This is represented by a 2×2 *truth or contingency table* as shown below:

	Left-handed True	Left-handed False
Blue-Eyed True	p_1	p_2
Blue-Eyed False	p_3	p_4

Table: GeneralTruth Table

Although there are four possible combinations of eye-color and handedness to be considered, the related probabilities are not completely independent of each other. We have the standard normalization requirement

$$\sum_i p_i = 1 \tag{3.124}$$

In addition, we also have two conditions on the so-called *marginal* probabilities

$$p_1+p_2 = prob(blue\cap left|I)+prob(blue\cap right|I) = 1/3 \quad (3.125)$$

$$p_1 + p_3 = prob(blue \cap left|I) + prob(not - blue \cap left|I) = 1/3 \quad (3.126)$$

Since any $p_i \geq 0$, these imply that $0 \leq p_1 \leq 1/3$. Using this result we can characterize the contingency table by a single variable $x = p_1$ as in the table below:

	Left-handed True	Left-handed False
Blue-Eyed True	$0 \leq x \leq 1/3$	$1/3 - x$
Blue-Eyed False	$1/3 - x$	$1/3 + x$

Table: For Kangaroo Problem

where we have used

$$x = p_1 \quad (3.127)$$

$$p_1 + p_2 = \frac{1}{3} \rightarrow p_2 = \frac{1}{3} - x \quad (3.128)$$

$$p_1 + p_3 = \frac{1}{3} \rightarrow p_3 = \frac{1}{3} - x \tag{3.129}$$

$$p_1 + p_2 + p_3 + p_4 = 1 \rightarrow p_4 = \frac{1}{3} + x \tag{3.130}$$

All such solutions, where $0 \leq x \leq 1/3$, satisfy the constraints of the testable information that is available. Which one is best?

Common sense leads us towards the assignment based on independence of these two traits, that is, any other assignment would indicate a knowledge of kangaroo eye-color told us something about its handedness. Since we have no information to determine even the sign of any potential correlation, let alone its magnitude, any choice other than independence is not justified.

The independence choice says that

$$x = p_1 = prob(blue \cap left|I) = prob(blue|I)prob(left|I) = \frac{1}{9} \tag{3.131}$$

In this particular example it was straightforward to decide the most sensible pdf assignment in the face of the inadequate information.

We now ask whether there is some function of the $\{p_i\}$ which, when maximized subject to the known constraints, yields the *independence* solution. The importance of finding an answer to this question is that it would become a good candidate for a general *variational principle* that could be used in situations that were too complicated for our common sense.

Skilling has shown that the only function which gives $x = 1/9$ is the entropy S as specified above or

$$S = -\sum_{i=1}^{4} p_i \log_e(p_i) \tag{3.132}$$

$$= -x \log_e(x) - 2\left(\frac{1}{3} - x\right) \log_e\left(\frac{1}{3} - x\right) - \left(\frac{1}{3} + x\right) \log_e\left(\frac{1}{3} + x\right)$$

The results of Skilling's investigations, including three proposed alternatives,

$$S1 = -\sum_{i=1}^{4} p_i \log_e(p_i) \Rightarrow \text{MaxEnt}$$

$$S2 = -\sum_{i=1}^{4} p_i^2 \qquad S3 = -\sum_{i=1}^{4} \log_e(p_i) \qquad S4 = -\sum_{i=1}^{4} \sqrt{p_i} \tag{3.133}$$

is shown in the table below:

Function	Optimal x	Implied Correlation
S1	0.1111	None
S2	0.0833	Negative
S3	0.1301	Positive
S4	0.1218	Positive

Table: Skilling Results

Clearly, only the MaxEnt assumption leads to an optimal value with no correlations as expected.

Let us look at another example that lends further support to the MaxEnt principle.

The Team of Monkeys

Suppose there are M distinct possibilities $\{X_i\}$ to be considered. How can we assign truth tables ($prob(X_i|I) = p_i$) to these possibilities given some testable information I (experimental results).

What is the most honest and fair procedure?

Imagine playing the following game.

The various propositions are represented by different boxes all of the same size into which pennies are thrown at random.

The tossing job is often assigned to a team of monkeys under the assumption that this will not introduce any underlying bias into the process.

After a very large number of coins have been distributed into the boxes, the fraction found in each of the boxes gives a possible assignment of the probability for the corresponding $\{X_i\}$.

The resulting pdf may not be consistent with the constraints of I, of course, in which case it must be rejected as a potential candidate. If it is in agreement, then it is a viable option.

The process is then repeated by the monkeys many times. After many such trials, some distributions will be found to come up more often than others. The one that occurs most frequently (and satisfies I) would be a sensible choice for $prob(\{X_i\}|I)$.

This is so because the team of monkeys has no axe to grind (no underlying bias) and thus the most frequent solution can be regarded as the one that best represents our state of knowledge.

It agrees with all the testable information available while being as indifferent as possible to everything else.

Does this correspond to the pdf to the greatest value of $S = -\sum p_i \log_e(p_i)$?

After the monkeys have tossed all the pennies given to them, suppose that we find n_1 in the first box, n_2 in the second box, and so on. We then have

$$N = \sum_{i=1}^{M} n_i = \text{total number of coins} \tag{3.134}$$

which will be assumed to be very large and also much greater than the number of boxes M.

This distribution gives rise to the candidate pdf $\{p_i\}$ for the possibilities $\{X_i\}$:

$$p_i = \frac{n_i}{N} \quad , \quad i = 1, 2, \ldots, M \tag{3.135}$$

Since every penny can land in any of the boxes there are M^N number of different ways of tossing the coins among the boxes. Each way, by assumption of randomness and no underlying bias by the monkeys, is equally likely to occur. All of the basic sequences, however, are not distinct, since many yield the same distribution $\{n_i\}$. The expected frequency F with which a set $\{p_i\}$ will arise, is given by

$$F\left(\{p_i\}\right) = \frac{\text{number of ways of obtaining}\{n_i\}}{M^N} \tag{3.136}$$

The numerator is just the number of ways to distribute N coins in a distribution $\{n_i\}$ which is given by

$$\text{number of ways of obtaining}\{n_i\} = \frac{N!}{n_1!n_2!\ldots n_M!} \tag{3.137}$$

Putting everything together we have

$$F\left(\{p_i\}\right) = \frac{\text{number of ways of obtaining}\{n_i\}}{M^N} = \frac{\frac{N!}{n_1!n_2!\ldots n_M!}}{M^N} \tag{3.138}$$

$$\log(F) = -N\log(M) + \log(N!) - \sum_{i=1}^{M} \log(n_i!) \tag{3.139}$$

Using Stirling's approximation $\log(n_i!) \approx n\log(n) - n$ for large n, we find

$$\begin{aligned}\log(F) &= -N\log(M) + N\log(N) - \sum_{i=1}^{M} n_i \log(n_i) - N + \sum_{i=1}^{M} n_i \\ &= -N\log(M) + N\log(N) - \sum_{i=1}^{M} n_i \log(n_i) \end{aligned} \tag{3.140}$$

and thus

$$
\begin{aligned}
\log(F) &= -N\log(M) + N\log(N) - \sum_{i=1}^{M} p_i N \log(p_i N) \\
&= -N\log(M) + N\log(N) - \sum_{i=1}^{M} p_i N (\log(p_i) + \log(N)) \\
&= -N\log(M) + N\log(N) - N\sum_{i=1}^{M} p_i \log(p_i) \\
&\qquad - N\log(N)\sum_{i=1}^{M} p_i \\
&= -N\log(M) + N\log(N) - N\sum_{i=1}^{M} p_i \log(p_i) - N\log(N) \\
&= -N\log(M) - N\sum_{i=1}^{M} p_i \log(p_i) \qquad (3.141)
\end{aligned}
$$

Maximizing the $\log(F)$ is equivalent to maximizing F, which is the expected frequency with which the monkeys will come up with the candidate pdf $\{p_i\}$, that is, maximizing $\log(F)$ will give us the assignment $prob(\{X_i\}|I)$ which best represents our state of knowledge consistent with the testable information I. Since M and N are constants, this is equivalent to the constrained maximization of the entropy function.

$$S = -\sum p_i \log_e(p_i) \tag{3.142}$$

and so we recover the MaxEnt procedure once again.

3.5 **Discussion**

In discussions of Bayesian methods, opponents often use the words *subjective probabilities* to say that the methods are not as valid as normal *objective* probability theory.

These opponents are misguided.

The main point of concern centers around the choice of the prior pdf, that is, what should we do if it is not known?

This is actually a very strange question. It is usually posed this way by opponents of the Bayesian methods in an attempt to prove its subjective nature.

No probability, whether prior, likelihood or whatever, is ever *known*. It is simply an assignment which reflects the relevant information that is available. Thus, $prob(x|I_1) \neq prob(x|I_2)$, in general, where the conditioning statements I_1 and I_2 are different.

Nevertheless, objectivity can, and must, be introduced by demanding the two people with the same information I should assign the same pdf. I think that this consistency requirement is the most important idea of all.

Invariance arguments, under transformation groups, can be used to uniquely determine a pdf when given only the nature of the quantities involved. MaxEnt provides a powerful extension when we have testable constraints.

While we may yet be far from knowing how to convert every piece of vague information into a concrete probability assignment, we can deal with a wide variety of problems with these ideas.

The important point is that nowhere in our discussion have we explicitly differentiated between a prior and a likelihood. We have only considered how to assign $prob(X|I)$ for different types of I. If X pertains to data, then we call $prob(X|I)$ a likelihood. If neither X nor I refers to (new) measurements, then we may say it is a prior.

The distinction between the two cases is one of nomenclature and not of objectivity or subjectivity. If it appears otherwise, then this is because we are usually prepared to state conditioning assumptions for the likelihood function but shy away from doing likewise for the prior pdf.

The use of Bayesian methods in quantum mechanics presents a very different view of quantum probability than normally appears in quantum theory textbooks. It is becoming increasingly important in discussions of measurement.