

A small Handbook of Quantum Mechanics

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“Seek simplicity and distrust it.” . . . Alfred North Whitehead

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Chapter 1

Bras, Kets, Vector Spaces And All That

1.1 Introduction

This handbook is meant to be a short introduction to *Quantum Mechanics*. It is not meant to be complete nor rigorous. Rather it is meant to give an overview of the mathematical formalism in a conceptual way.

Among the major “discoveries” of physics in the twentieth century, we would surely have to include the following two laws:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$$

and

$$[\hat{x}, \hat{p}_x] = i\hbar.$$

What do they mean? Of what use are they?

1.1.1 An (imperfect, but perhaps useful) Analogy

Flip a coin into the air. As it falls, grab it in mid-air and slap it onto your wrist to determine if it is heads or tails. Do it again, as identically as possible.

Grabbing the coin from mid-air and slapping it onto your wrist is a “measurement” in which you interfere with the spinning coin to determine a measured “value”, heads or tails. There are only two possible outcomes of the measurement and the probability for each outcome is 50%. If someone asks

whether the coin is heads or tails while it is still in the air, there is no good answer, only possibility and probability. But you might think of the coin in the air as being in some kind of combination of the two possibilities. (To make this analogy more like a quantum system, imagine that you cannot see the coin while it is in the air and know nothing about its classical motion. In fact, all you know about the coin is the result of your measurement at the end of its fall. For that there are just two possibilities with equal probabilities.)

Quantum systems are like the coin. There is only *possibility* and *probability*.

1.2 Possibilities and Probabilities

A ket $|n\rangle$ is a symbol for a discrete *possibility state* of existence for a system. When the coin lies on your wrist, there are only two: heads up $|h\rangle$ and tails up $|t\rangle$.) After we make a measurement, we get one or the other and not in between, so that is a good enough reason to say that there are just two *possibility states*. (If the possibility states were to correspond to a smooth continuity of possibilities, then $|\xi\rangle$ represents one of a continuous set of possibility states with ξ labeling these possibilities.)

A ket $|\psi\rangle$ represents a more general state. A state is a symbol for the existence of some physical system. (The symbol $|\psi\rangle$ might represent the system of the coin while still in mid-air.) The possibility states $|n\rangle$ are a special kind of states (sometimes called *determinate states*) that the system assumes as a consequence of the measurement. Do not confuse the possibility states with the actual measured values that result from a measurement. The labels inside the possibility kets identify the measured values associated with the respective state. As the coin moves in the air it is continually changing from one state to the other even though you would not ascribe a specific measured “value” of heads or tails until you actually made a measurement by catching it. At that point, the system (almost magically) changes from the general state to one or the other of the possibility states. A general state in particular is a very abstract thing, an ethereal symbol for existence, a mixture of many possibilities. Measured values are very concrete things. They are usually numbers that you get from a readout of a measuring instrument.

In quantum mechanics possibility states become the basis vectors for a vector space. General states are represented by a vector sum of possibility

states with complex numbers as coefficients:

$$|\psi\rangle = \sum_n c_n |n\rangle + \int_{\xi_1}^{\xi_2} c(\xi) |\xi\rangle d\xi$$

The real numbers $|c_n|^2$ and $|c(\xi)|^2$ are where we put the *probabilities*. If you make a series of measurements, each on an identically prepared state, the probabilities $|c_n|^2$ tell you with which probability you will get each one of the possible measured values for the possibilities as the result of your measurements. For our coin,

$$|\psi\rangle = \frac{\sqrt{2}}{2} |h\rangle + \frac{\sqrt{2}}{2} |t\rangle,$$

so that the probability of each possibility is 1/2.

Linear operators change a vector (or *map* it) into some other vector by some prescription. This can be expressed for an operator \hat{A} by,

$$|v\rangle = \hat{A} |u\rangle,$$

i.e., the operator \hat{A} changes or better, maps, $|u\rangle$ into $|v\rangle$. Physically interesting features of a system (position, momentum, energy, angular momentum) that can be made the subject of measurement are represented in the theory by operators ($\hat{x}, \hat{p}, \hat{H}, \hat{L}_z$).

Operators typically have special states associated with them. These special states are called the *eigenstates* of the operator. When an operator operates on an eigenstate (or eigenket), it spits back the eigenket multiplied by a number (called the *eigenvalue*) according to,

$$\hat{A} |n\rangle = a_n |n\rangle.$$

In general, the eigenvalue is a complex number. However, a special class of operators have only real numbers as their eigenvalues. These operators are called *Hermitian operators*. The real eigenvalues a_n of Hermitian operators then become the set of possible measured values that a measurement of a physical quantity associated with the operator \hat{A} can yield when a measurement is performed on an arbitrary state $|\psi\rangle = \sum_n c_n |n\rangle$. In this case the eigenstates of \hat{A} are the possibility states. Note that the possibility states are the eigenstates, but the actual results of measurement (the possibilities) are the eigenvalues.

If a measurement of some physical characteristic of a general state is made, one gets some measured value, one of the eigenvalues of the operator \hat{A} that the theory associates with the measurement. But it is the strange truth of quantum systems that making an identical measurement on the exact same system will not necessarily yield the same measured value. Each possibility has its own probability. After many measurements of the quantity associated with the operator \hat{A} are made of the identical system $|\psi\rangle$, one would have enough numbers to calculate an average value. This average value is called the *expectation value* of the measurement and is given the symbol $\langle \hat{A} \rangle$. With $|c_n|^2$ as the probabilities and a_n being the possibilities, we should work things out so that,

$$\langle \hat{A} \rangle = \sum_n |c_n|^2 a_n.$$

Can we make all of this work in an orderly and systematic way?

1.3 The Dual Space of Bras

A vector space needs an *inner product*, if for no other reason than to define a *norm* for a vector. In familiar three-space, the inner product of two vectors is called a *dot product*. The dot product of a 3-vector with itself yields the square of its length. In the vector space of kets, it is desirable for the possibility states to act like unit vectors in three-space, i.e., each to have a norm of 1. Because the admissible numbers c_n are complex, the definition of a norm is somewhat more involved in the vector space of possibility states than it is in familiar 3-space of vectors with real coefficients.

To define an inner product of two kets, we need a second vector space, called the *bra space*. Bras are the basis vectors for bra space, but they are not possibility states at all. A bra $\langle u|$ is a symbol for an operation that is to be performed on a ket to generate a complex number as a consequence. Thus a bra maps a particular ket on which it operates onto a complex number.

Reverting to familiar 3-space in which there are unit vectors \hat{e}_1 , \hat{e}_2 , and, \hat{e}_3 , consider the following definition of an operation: "Take a dot product of \hat{e}_1 with ...". The operation is to be performed on some vector, yet unspecified. The symbol for this operation might be written

$$\langle 1| \equiv \hat{e}_1 \bullet .$$

If the operation $\langle 1|$ is performed on an arbitrary vector, it might look like this:

$$\hat{\mathbf{e}}_1 \bullet (a_1 \hat{\mathbf{e}}_1 + a_2 \hat{\mathbf{e}}_2 + a_3 \hat{\mathbf{e}}_3) = a_1$$

or in this newer notation,

$$\langle 1| \bullet (a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle) = a_1$$

if the unit vectors are orthonormal.

The bra operations can themselves form a vector space. For example, we can add the operations,

$$\langle u| = b_1 \langle 1| + b_2 \langle 2|$$

where b_1 and b_2 are real numbers in our 3-d example. We then have the possible operation,

$$(b_1 \langle 1| + b_2 \langle 2|) \bullet (a_1 |1\rangle + a_2 |2\rangle + a_3 |3\rangle) = b_1 a_1 + b_2 a_2,$$

i.e., when the operation is performed on a vector, it spits out a real number. (We will dispense with the \bullet in our notation from here on.)

The dual space for our ket space is defined similarly, except that the operation of a bra on a ket generates a complex number rather than a real number. The symbol for the complex number generated when a bra $\langle u|$ acts on a ket $|v\rangle$ is $\langle u|v\rangle$. For each ket $|v\rangle = c_1 |1\rangle + c_2 |2\rangle$ in ket space, there is a corresponding bra $\langle v| = c_1^* \langle 1| + c_2^* \langle 2|$ in bra space (called its *conjugate*), such that

$$\langle v|v\rangle = |c_1|^2 + |c_2|^2$$

is a real number (no imaginary part in this case) and serves as the norm of the ket. The inner product of the ket $|u\rangle$ with $|v\rangle$ is the complex number $\langle u|v\rangle$. To make the norms come out real, the bra that goes with $|v\rangle = c_1 |1\rangle + c_2 |2\rangle$ has to be $\langle v| = c_1^* \langle 1| + c_2^* \langle 2|$ so that $\langle v|v\rangle$ is real. The use of the complex conjugates c_1^* and c_2^* in the bra space is said to be an *antilinear* relationship between $\langle v|$ and $|v\rangle$.

Just as c and c^* are complex conjugates of one another, $|v\rangle$ and $\langle v|$ are said to be conjugates of one another. Operators also have conjugates (called *Hermitian conjugates*.) Thus, the conjugate of \hat{A} is \hat{A}^\dagger and the conjugate of $|v\rangle = \hat{A}|u\rangle$ is defined from $\langle v| = \langle u| \hat{A}^\dagger$.

However, an operator \hat{A} can also operate in the bra space although it does not give the bra $\langle v|$ defined above. Rather, another bra $\langle w|$ is produced, not $\langle v|$, according to

$$\langle w| = \langle u| \hat{A}$$

such that for any $|\eta\rangle$

$$\langle w|\eta\rangle = (\langle u|\hat{A})|\eta\rangle = \langle u|(\hat{A}|\eta\rangle).$$

Thus, if $A|\eta\rangle$ and the conjugate of $|u\rangle$ are defined, then \hat{A} has a defined action in the bra space in just such a way that the parens are not needed. The operator \hat{A} can be thought of as able to operate to the right or to the left:

$$(\langle u|\hat{A})|\eta\rangle = \langle u|(\hat{A}|\eta\rangle) = \langle u|\hat{A}|\eta\rangle.$$

The dual space is constructed in a fiendishly clever way. Here are the rules:

Conjugates:

$$\begin{aligned} c_n &\text{ and } c_n^* \\ |v\rangle &\text{ and } \langle v| \\ \hat{A} &\text{ and } \hat{A}^\dagger. \end{aligned}$$

To create the conjugate of a bra-ket expression, reverse the order of all elements, change explicit complex numbers into their complex conjugates, change all operators into their Hermitian conjugates. Thus, the Hermitian conjugate of the operator

$$\hat{A}\hat{B}|u\rangle\langle v|\hat{C}$$

is

$$\hat{C}^\dagger|v\rangle\langle u|\hat{B}^\dagger\hat{A}^\dagger.$$

The complex conjugate of the complex number

$$\langle t|\hat{A}\hat{B}|u\rangle\langle v|\hat{C}|w\rangle$$

is

$$\langle w|\hat{C}^\dagger|v\rangle\langle u|\hat{B}^\dagger\hat{A}^\dagger|t\rangle.$$

The (complex) conjugate of the complex number

$$\langle u|\hat{A}|v\rangle$$

is

$$\langle u|\hat{A}|v\rangle^* = \langle v|\hat{A}^\dagger|u\rangle.$$

In order for the $|c_n|^2$ in the expression $|v\rangle = \sum c_n |n\rangle$ to qualify as probabilities, the sum of the probabilities for all possibilities must be one. Thus, possibility states are constructed to be *orthonormal*, i.e.,

$$\langle m|n\rangle = \delta_{mn}$$

where δ_{mn} is the *Kronecker delta* (1 if $m = n$, but 0 otherwise). Then if the ket

$$|v\rangle = \sum c_n |n\rangle$$

is also normalized to 1, we have,

$$\langle v|v\rangle = \left(\sum_n c_n^* \langle n|\right) \left(\sum_m c_m |m\rangle\right) = \sum_n \sum_m c_n^* c_m \delta_{nm} = \sum_n |c_n|^2 = 1$$

and the individual $|c_n|^2$ can be interpreted as probabilities for each possibility that is enumerated by n since the sum of probabilities for all possibilities must be 1.

If possibility states are continuous rather than discrete, the Kronecker delta normalization is replaced with the *Dirac delta function* $\delta(\xi' - \xi)$

$$\langle \xi'|\xi\rangle = \delta(\xi' - \xi),$$

defined to be zero if $\xi' - \xi \neq 0$ and infinite otherwise in such a way that

$$\int \delta(\xi' - \xi) d\xi' = 1,$$

and,

$$\int \delta(\xi' - \xi) f(\xi') d\xi' = f(\xi)$$

(given that the integral is over an interval including ξ .) If,

$$|v\rangle = \int_{\xi_1}^{\xi_2} c(\xi) |\xi\rangle d\xi,$$

then,

$$\int_{\xi_1}^{\xi_2} |c(\xi)|^2 d\xi = 1.$$

General states may have a mixture of discrete and continuous possibility states.

Chapter 2

Operators

2.1 Hermitian Operators

In quantum mechanics, operators are associated with measurable quantities (although not exclusively so) called *observables*. Thus a measured value of the x -component of momentum is associated somehow with the \hat{p}_x operator, the measured value of energy with the Hamiltonian operator \hat{H} and the measured value of the z -component of angular momentum with the operator \hat{L}_z .

But a measurement is also defined and limited by the possibilities. How are the possibilities related to the operator?

Operators have *eigenkets* defined by,

$$\hat{A} |n\rangle = a_n |n\rangle .$$

(For simplicity we are assuming discrete eigenkets, of which there may be many, and associated a_n .) Basically, this expression says that if you operate with the operator \hat{A} on an eigenket, the state is essentially undisturbed except for producing the factor a_n . In the theory, the *eigenvalue* a_n becomes a possible measured value of the quantity associated with \hat{A} . If you repeat a measurement on an identically prepared system, you get one of the set of possible a_n each time.

However, the measured value must be some real quantity, not a complex number. The measured values of energy and position and angular momentum are all real numbers. In order for this to be so, measurable quantities must be associated with a special kind of linear operator called a *Hermitian operator*.

A Hermitian operator is an operator that is its own Hermitian conjugate, i.e., $\hat{A} = \hat{A}^\dagger$.

Hermitian operators have some very useful properties. The eigenvalues a_n of a Hermitian operators are all real and the eigenkets $|n\rangle$ provide a complete basis for spanning a vector space. Indeed, the eigenkets are just the “possibility states” that we have pointed to from the beginning. The Hamiltonian operator \hat{H} and the angular momentum operator \hat{L}_z are Hermitian operators.

Consider a state $|\psi\rangle = \sum_n c_n |n\rangle$ of the system such that $\langle\psi|\psi\rangle = 1$, and where the possibility states $|n\rangle$ are the eigenkets of the ideal measurement operator \hat{A} .

This is what happens when we operate on a general state $|\psi\rangle$ with the operator \hat{A} :

$$\hat{A}|\psi\rangle = \hat{A}\left(\sum_n c_n |n\rangle\right) = \sum_n a_n c_n |n\rangle.$$

Clearly, the operator has created a new ket, but it is not evident what its significance might be. However, if we form $\langle\psi|\hat{A}|\psi\rangle$,

$$\begin{aligned} \langle\psi|\hat{A}|\psi\rangle &= \left(\sum_m c_m^* \langle m|\right) \hat{A} \left(\sum_n c_n |n\rangle\right) \\ &= \sum_m \sum_n c_m^* c_n \langle m|\hat{A}|n\rangle \\ &= \sum_m \sum_n a_n \delta_{mn} c_m^* c_n \\ &= \sum_m a_m |c_m|^2. \end{aligned}$$

But the factors $|c_m|^2$ are the probabilities for each measured value a_m , or in other words, we have calculated the *average value* that one would expect if we repeated measurements over and over again on an identically prepared system. We will denote the average value for the measurement corresponding to \hat{A} on a system in general state $|\psi\rangle$ as

$$\langle A \rangle = \langle\psi|\hat{A}|\psi\rangle.$$

Because we have used a Hermitian operator \hat{A} , we are assured that its eigenvalues a_n are real and that the average value we thus obtain is a real (not complex) number as an average value for ideal measurement must be. This average value $\langle\hat{A}\rangle$ is called the *expectation value* of the measurement.

What is special about the eigenstates $|n\rangle$? For a system that is in an eigenstate $|n\rangle$ of \hat{A} ,

$$\langle \hat{A} \rangle = \langle n | \hat{A} | n \rangle = a_n \langle n | n \rangle = a_n.$$

If the system is in such an eigenstate, a measurement always gives the same measured value (possibility) with probability one.

2.2 Operators of the form $|u\rangle \langle v|$

A useful kind of (non-Hermitian) operator takes the form $\hat{O} = |u\rangle \langle v|$ or, using discrete possibility states, $|m\rangle \langle n|$. (Continuous possibility states can be handled analogously.) If the latter operates on a state $|v\rangle$, it produces a new ket,

$$|m\rangle \langle n | v \rangle.$$

Since the symbol $\langle n | v \rangle$ is just a complex number, the new ket takes the form $c |m\rangle$.

A particularly useful operator of this form, that does absolutely nothing to a vector that it operates on, is the *identity operator* \hat{I} that consists of a sum over all possibility states of the form,

$$\hat{I} = \sum_n |n\rangle \langle n|$$

or, if the possibilities are continuous,

$$\hat{I} = \int_{\xi_1}^{\xi_x} |\xi\rangle d\xi \langle \xi|.$$

If the possibility states are discrete and complete, then an arbitrary state can be expressed,

$$|\psi\rangle = \sum_n c_n |n\rangle$$

and,

$$\hat{I} |\psi\rangle = \left(\sum_m |m\rangle \langle m| \right) \sum_n c_n |n\rangle = \sum_m \sum_n \delta_{mn} c_n |m\rangle = \sum_m c_m |m\rangle = |\psi\rangle.$$

While this latter example seems uselessly simple, it has some unexpected utility.

Chapter 3

Representations

The symbol $|\psi\rangle$ is a symbol for some system (imagine an atom, for example). Perhaps you would like to know the precise position x of the system, what its momentum p_x is, what its energy E is and what the z -component of its angular momentum is. Each measurement requires an experimental set up. Can you get enough equipment positioned around the atom to measure all of these things simultaneously?

The answer turns out to be: no. There are some kinds of measurements that are inconsistent with others. You can know the position x of the system, but not simultaneously its momentum p_x . But you may be able to measure the energy of the system and the z -component of its angular momentum simultaneously. How do you know which you can and which you can't?

In quantum mechanics measurements are associated with operators. Possibility states are the eigenvectors of the operators. Possible measured values are the eigenvalues of the operators. Under what conditions can you find eigenvectors that are simultaneously the eigenvectors of two different operators?

The answer lies in the *commutator*

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

of the two operators. If two operators commute, it is possible to find eigenstates that serve for both simultaneously, but if they do not commute, it is not possible. For measurement, this means that if two operators do not commute, it is not possible to measure both corresponding physical features of the system simultaneously. Since,

$$[\hat{x}, \hat{p}_x] = i\hbar,$$

it is not possible to measure both x and p_x simultaneously, but if

$$[\hat{H}, \hat{L}_z] = 0$$

it would be possible to obtain a simultaneous measurement of E and L_z . For our system symbolized by $|\psi\rangle$ it means that you could measure x or you could measure p_x , but you would need separate experiments to do it.

Now each of the operators nevertheless has its own eigenvectors and eigenvalues. Each provides a set of possibility states that we could use as basis states. Let's take two: continuous eigenstates of position $|x\rangle$ and discrete eigenstates $|E_n\rangle$ of energy. We could write,

$$|\psi\rangle = \int_{-\infty}^{+\infty} c(x') |x'\rangle dx'$$

or,

$$|\psi\rangle = \sum_n c_n |E_n\rangle,$$

since $|\psi\rangle$ is, in both cases, the symbol for the same system.

Consider doing an inner product of $|\psi\rangle$ and an eigenfunction of the energy operator (the Hamiltonian),

$$\langle E_m | \psi \rangle = \langle E_m | \left(\sum_n c_n |E_n\rangle \right) = \sum_n c_n \delta_{mn} = c_m.$$

What we get for all possible choices of m are an ordered set of complex numbers, c_m . We could think of them as the elements of a very long column vector that is said to be a *representation* of the state $|\psi\rangle$ in the same way that the components a_i of an ordinary 3-vector \mathbf{a} are a representation of the 3-vector. (In another coordinate system with different basis vectors, a rotated coordinate system, the representation by components is a different set a'_i of numbers.)

But, we could also form,

$$\langle x | \psi \rangle = \langle x | \left(\int_{-\infty}^{+\infty} c(x') |x'\rangle dx' \right) = \int_{-\infty}^{+\infty} c(x') \delta(x - x') dx' = c(x).$$

This set of complex numbers could also be thought of as sitting in a tall column vector, but the elements are a continuous function of x . We call that complex function of x the *wave function* and denote it by

$$\psi(x) \equiv \langle x | \psi \rangle = c(x).$$

It is said to be the *position representation* of the state $|\psi\rangle$ and is usually referred to as the *wave function*.

Bras have representations as well. Consider $\langle\psi|x\rangle = (\langle x|\psi\rangle)^*$. Put these complex conjugate numbers in a row vector. The row vector is said to be the *position representation* of the bra $\langle\psi|$. If the numbers that go into the representation of $|\psi\rangle$ are given by $\psi(x)$, then the numbers that go into the representation of $\langle\psi|$ are given by $\psi^*(x)$. In terms of the representations of $\langle\psi|$ and $|\psi\rangle$, the norm of the state $\langle\psi|\psi\rangle$ is just the matrix product of the respective row vector and the column vector.

In a similar fashion we can create momentum representations (using eigenstates of \hat{p}_x) and angular momentum representations (using eigenstates of \hat{L}_z -component) of the self-same state $|\psi\rangle$. And since we are now dealing with numbers rather than abstract states, we can start to use more familiar tools of mathematics.

Operators also have representations. Operators are represented by matrices of (usually) complex numbers created by expressions such as,

$$\langle m|\hat{A}|n\rangle$$

for a discrete basis set, and

$$\langle\xi'|\hat{A}|\xi\rangle$$

for a continuous possibility basis set. If you think of $\langle m|\psi\rangle$ as being arranged in a column vector and $\langle n|\hat{A}|m\rangle$ being the elements of a matrix with rows enumerated by n and columns by m , the representation of $|\phi\rangle = \hat{A}|\psi\rangle$ is a column vector obtained by multiplying the matrix for \hat{A} times the column vector for $|\psi\rangle$. Indeed, using the identity operator \hat{I} ,

$$\hat{I} = \sum_m |m\rangle\langle m|$$

we get,

$$|\phi\rangle = \hat{A}|\psi\rangle = \hat{A}\hat{I}|\psi\rangle = \hat{A}\sum_m |m\rangle\langle m|\psi\rangle.$$

Now form the representation of $|\phi\rangle$ yielding,

$$\langle n|\phi\rangle = \sum_m \langle n|\hat{A}|m\rangle\langle m|\psi\rangle.$$

This is just another way of writing the matrix multiplication indicated.

If the basis state for the representation is just the set of eigenvectors of \hat{A} , the matrix representation of \hat{A} is particularly simple because,

$$\langle n | \hat{A} | m \rangle = a_m \delta_{nm}$$

i.e., the matrix representing \hat{A} is just a diagonal matrix with the eigenvalues of \hat{A} on the diagonal.

The *position representation* is a continuous representation of particular interest, for which we use the eigenstates of position $|x\rangle$, satisfying,

$$\hat{x} |x\rangle = x |x\rangle$$

$$\langle x | x' \rangle = \delta(x - x')$$

$$\langle x | \hat{x} | x' \rangle = x' \delta(x - x').$$

The momentum operator \hat{p}_x has a position representation that can be derived from the commutator relationship $[\hat{x}, \hat{p}_x] = i\hbar$ and the properties of the Dirac delta function (summarized in a separate chapter of this handbook). On the one hand,

$$\langle x' | [\hat{x}, \hat{p}_x] | x \rangle = i\hbar \langle x' | x \rangle = i\hbar \delta(x' - x).$$

On the other hand,

$$\langle x' | [\hat{x}, \hat{p}_x] | x \rangle = \langle x' | \hat{x} \hat{p}_x - \hat{p}_x \hat{x} | x \rangle = (x' - x) \langle x' | \hat{p}_x | x \rangle.$$

Equating,

$$(x' - x) \langle x' | \hat{p}_x | x \rangle = i\hbar \delta(x' - x).$$

However, the derivative of the Dirac delta function satisfies,

$$(x' - x) \delta'(x' - x) = -\delta(x' - x),$$

allowing us to conclude the very important result,

$$\langle x' | \hat{p}_x | x \rangle = -i\hbar \delta'(x' - x).$$

Turning finally to

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle = \left(\frac{\hat{p}_x^2}{2m} + \hat{V} \right) |\psi\rangle,$$

we express it in the position representation by forming the inner product of the equation with $|x\rangle$,

$$i\hbar \frac{\partial}{\partial t} \langle x|\psi\rangle = \langle x|\frac{\hat{p}_x^2}{2m}|\psi\rangle + \langle x|\hat{V}|\psi\rangle.$$

If the operator \hat{V} is itself only a function of the operator \hat{x} , the latter can operate to the left (generating eigenvalues x), yielding,

$$\langle x|\hat{V}|\psi\rangle = V(x)\langle x|\psi\rangle = V(x)\psi(x).$$

That leaves essentially (putting the identity operator \hat{I} to good use),

$$\begin{aligned} \langle x|\hat{p}_x\hat{p}_x|\psi\rangle &= \langle x|\hat{p}_x\hat{I}\hat{p}_x\hat{I}|\psi\rangle \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \langle x|\hat{p}_x|x'\rangle \langle x'|\hat{p}_x|x''\rangle \langle x''|\psi\rangle dx'dx'' \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} [-i\hbar\delta'(x-x')][-i\hbar\delta'(x'-x'')] \langle x''|\psi\rangle dx'dx''. \end{aligned}$$

Perform the integrals one at a time, using the Dirac delta function relationships (watch the minus signs!),

$$\int_{-\infty}^{+\infty} \delta'(x-x_0)f(x)dx = -f'(x_0),$$

and,

$$\delta'(x-x_0) = -\delta'(x_0-x)$$

to yield the *Schroedinger wave equation*

$$i\hbar \frac{\partial\psi(x)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x).$$

Chapter 4

Summary

Physical systems (atoms, molecules, etc.) exist in *states* of being symbolized by $|\psi\rangle$. The many possible states of a system can be made to form an abstract vector space.

Measurements (of position, momentum, energy, etc.) can be made on systems, but experience shows that measurements on identically prepared systems do not necessarily give the same measured value and, moreover, sometimes the measured values come in discrete possibilities. Thus, there is only *possibility* and *probability*.

For each kind of measurement there exists a linear *Hermitian operator* (for example, \hat{A}) that operates in the abstract vector space of states. Each of the Hermitian operators (for position, momentum, energy, etc.) has real eigenvalues a_n and corresponding eigenstates $|n\rangle$. The set of eigenvalues (the *spectrum*) is the set of all possible measured values for the measurement associated with the operator. These are the *possibilities*.

The eigenstates of each Hermitian operator $|n\rangle$, can be made mutually orthogonal and normalized to unity. These serve, like unit vectors in ordinary 3-space, as basis vectors for the abstract vector space. Each general state can also be normalized and can be represented as an expansion in one of these basis sets,

$$|\psi\rangle = \sum_n c_n |n\rangle.$$

The *probability* for obtaining the eigenvalue a_n as a result of a measurement of the system $|\psi\rangle$ is the real number $|c_n|^2$. The average value (*expectation value*) for identical measurements of identically prepared systems

is

$$\langle \hat{A} \rangle = \sum_n |c_n|^2 a_n.$$

The Law of Evolution of states is

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H} |\psi\rangle$$

where \hat{H} is the Hamiltonian (Energy) operator.

The complementary nature of position and momentum is expressed by

$$[\hat{x}, \hat{p}_x] = i\hbar.$$

This law institutes in the theory the feature that one cannot simultaneously measure precisely for a system both the position and its corresponding component of momentum.

Various *representations* can be made of the abstract vector space. In the *position representation*, the Law of Evolution of states (for a potential V depending only on position) is given in one dimension by *Schroedinger's Equation*

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x)\psi(x, t).$$

Chapter 5

Summary of Quantum Equations

1. Schroedinger's Law

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle$$

2. Canonical Commutation Relation

$$[\hat{x}, \hat{p}] = i\hbar$$

3. Schroedinger's Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad \text{---} > \quad -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi$$

4. Probability of finding a particle between a and b , at time t .

$$\int_a^b |\Psi(x, t)|^2 dx$$

5. Normalization

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1$$

6. Expectation value of x .

$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\Psi(x, t)|^2 dx$$

7. Expectation value of p_x .

$$\langle p_x \rangle = m \frac{d\langle x \rangle}{dt} = \int \left(\Psi^* \left[-i\hbar \frac{\partial}{\partial x} \right] \Psi \right) dx$$

8. Expectation value (general).

$$\langle Q(x, p) \rangle = \int \left(\Psi^* \left[Q(x, -i\hbar \frac{\partial}{\partial x}) \right] \Psi \right) dx$$

9. Uncertainty Principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

10. Generalized Uncertainty Principle

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2$$

11. Time Independent Schroedinger Equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

12. General Solution

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x, t).$$

13. Simple Harmonic Oscillator

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

$$\begin{aligned}
a_{\pm} &\equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x) \\
\psi_0(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \\
\psi_n(x) &= A_n(a_+)^n \psi_0(x) \\
a_+ \psi_n &= \sqrt{n+1} \psi_{n+1}, \quad a_- \psi_n = \sqrt{n} \psi_{n-1} \\
\psi_n &= \frac{1}{\sqrt{n!}} (a_+)^n \psi_0
\end{aligned}$$

14. Plancherel's Theorem

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk \iff F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$$

15. Schwarz Inequality

$$|\langle \alpha | \beta \rangle|^2 \leq |\langle \alpha | \alpha \rangle|^2 |\langle \beta | \beta \rangle|^2$$

16. Evolution of Expectation Value

$$\frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{Q}] \rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle$$

17. Generalized Time-Energy Uncertainty Principle

$$\sigma_H \sigma_Q \geq \frac{\hbar}{2} \left| \frac{d \langle Q \rangle}{dt} \right|$$

18. Spherical Harmonics

$$Y_{\ell}^m(\theta, \phi) = A P_{\ell}^m(\theta) e^{im\phi}$$

These are normalized to unity,

$$\int_0^{2\pi} \int_0^{\pi} [Y_{\ell}^m(\theta, \phi)]^* [Y_{\ell'}^{m'}(\theta, \phi)] \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'},$$

by choosing the normalization constant A to be

$$A = \epsilon \sqrt{\frac{2(\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!}}$$

$$\epsilon = (-1)^m, \quad m \geq 0$$

$$\epsilon = 1, \quad m < 0.$$

19. Hydrogen Solutions

Summarizing, normalized solutions to Schroedinger's equation for hydrogen-like atoms are:

$$\psi_{n\ell m} = \sqrt{\left(\frac{2Z}{na'_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+1)!]^3}} e^{-Zr/na'_0} \left(\frac{2Zr}{na'_0}\right)^\ell [L_{n-\ell-1}^{2\ell+1}(2Zr/na'_0)] Y_\ell^m(\theta, \phi),$$

$$\int \psi_{n\ell m}^* \psi_{n'\ell'm'} r^2 \sin\theta dr d\theta d\phi = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'},$$

where the reduced mass m_r is given by

$$m_r = \frac{m_e M}{(m_e + M)} = \frac{m_e}{(1 + m_e/M)} \approx m_e,$$

the Bohr radius is,

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2},$$

the Bohr radius corrected for the reduced mass is,

$$a'_0 = a_0(1 + m_e/M)$$

and the energy eigenvalues are,

$$E_n = -\frac{m_r Z^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} = -\frac{1}{2} \alpha^2 (m_e c^2) \left(1 + \frac{m_e}{M}\right)^{-1} \frac{Z^2}{n^2}.$$

the charge on the electron is e , the charge on the nucleus is Ze , the mass of the electron is m_e , the mass of the nucleus is M and the fine structure constant is α .

$$E_0 = -\frac{1}{2} \alpha^2 (m_e c^2) = -13.6 \text{ eV}.$$

The integer n takes the values $n = 1, 2, \dots, \infty$. The integer ℓ takes values $\ell = 0, \dots, n-1$ and the index m take values $m = \ell, -\ell + 1, \dots, \ell - 1, \ell$.

20. Angular Momentum

$$[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$$

$$\begin{aligned}
\hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \\
[\hat{L}^2, \hat{L}_i] &= 0 \\
\hat{L}_\pm &\equiv \hat{L}_x \pm i\hat{L}_y \\
\hat{L}_+ \hat{L}_- &= \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z \\
\hat{L}_- \hat{L}_+ &= \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z \\
\hat{L}_\pm |\ell m\rangle &= \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)} |\ell m \pm 1\rangle \\
\hat{L}^2 |\ell, m\rangle &= \hbar^2\ell(\ell+1) |\ell, m\rangle, \quad \hat{L}_z |\ell, m\rangle = m\hbar |\ell, m\rangle \\
\hat{L}^2 - \dots &> -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \\
\hat{L}_z - \dots &> -i\hbar \frac{\partial}{\partial\phi}
\end{aligned}$$

21. Pauli Spin Matrices

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

22. Triplet, Singlet States

$$\left\{ \begin{array}{l} |11\rangle = |\uparrow\uparrow\rangle \\ |10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |1-1\rangle = |\downarrow\downarrow\rangle \end{array} \right\} \quad s = 1 \text{ (triplet)}$$

$$\left\{ |00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right\} \quad s = 0 \text{ (singlet)}$$

23. Symmetrization Requirement

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \pm\psi(\mathbf{r}_2, \mathbf{r}_1)$$

24. Statistics

$$n(\epsilon) = \begin{cases} e^{-(\epsilon-\mu)/k_bT} & \text{Maxwell - Boltzmann} \\ \frac{1}{e^{(\epsilon-\mu)/k_bT} + 1} & \text{Fermi - Dirac} \\ \frac{1}{e^{(\epsilon-\mu)/k_bT} - 1} & \text{Bose - Einstein} \end{cases}$$

25. Planck's Blackbody Spectrum

$$\rho(\omega) = \frac{\hbar\omega^3}{\pi^2 c^2 (e^{\hbar\omega/k_bT} - 1)}$$

Chapter 6

All You Need To Know About Commutators

$$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

$$[\hat{A}, \hat{A}] = 0$$

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{C}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{C}, \hat{A}]] = 0$$

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$$

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$$

$$[\hat{L}_i, \hat{x}_j] = i\hbar\epsilon_{ijk}\hat{x}_k$$

$$[\hat{L}_i, \hat{p}_j] = i\hbar\epsilon_{ijk}\hat{p}_k$$

$$[\hat{L}^2, \hat{L}_z] = 0$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$\epsilon_{ijk} = 1$, even permutation, ijk

$\epsilon_{ijk} = -1$, odd permutation, ijk

$\epsilon_{ijk} = 0$, otherwise

Chapter 7

Useful Mathematical Formulas

Integrals

$$\int_0^{\infty} x^n e^{-x/a} dx = n! a^{n+1}$$

$$\int_0^{\infty} x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi} \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1}$$

$$\int_0^{\infty} x^{2n+1} e^{-x^2/a^2} dx = \frac{n!}{2} a^{2n+2}$$

$$\frac{2}{a} \int_0^a \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a} dx = \delta_{mn}$$

$$\int x \sin(ax) dx = \frac{1}{a^2} \sin(ax) - \frac{x}{a} \cos(ax)$$

$$\int x \cos(ax) dx = \frac{1}{a^2} \cos(ax) + \frac{x}{a} \sin(ax)$$

$$\int_a^b f \frac{dg}{dx} dx = - \int_a^b \frac{df}{dx} g dx + fg|_a^b$$

Trigonometry

$$\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b$$

$$\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$$

$$c^2 = a^2 + b^2 - 2ab \cos \theta$$

Taylor's Expansion

For x near x_0 ,

$$f(x) = f(x_0) + \left(\frac{df}{dx}\right)_0 (x - x_0) + \dots + \frac{1}{n!} \left(\frac{d^n f}{dx^n}\right)_0 (x - x_0)^n + \dots$$

Chapter 8

All You Need to Know About the Dirac Delta Function

The Dirac delta function is defined by

$$\delta(x - x_0) = \begin{cases} 0 & \text{if } x \neq x_0 \\ +\infty & \text{if } x = x_0 \end{cases}$$

such that,

$$\int_{-\infty}^{+\infty} \delta(x - x_0) dx = 1.$$

The main properties of the function $\delta(x)$ are the following:

$$\int_{-\infty}^{+\infty} f(x)\delta(x - x_0)dx = f(x_0)$$

$$\delta(x) = \delta(-x)$$

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

$$x\delta(x) = 0$$

$$f(x)\delta(x - x_0) = f(x_0)\delta(x - x_0)$$

$$\int \delta(x - y)\delta(y - a)dy = \delta(x - a)$$

If $g(x)$ and $g'(x)$ never vanish simultaneously and $g(x_n) = 0$, then

$$\delta[g(x)] = \sum_n \frac{1}{|g'(x_n)|} \delta(x - x_n).$$

The function $\delta(x)$ is differentiable to all orders. Its m th derivative $\delta^{(m)}(x)$ is defined by the property,

$$\int_{-\infty}^{+\infty} \delta^{(m)}(x - x_0) f(x) dx = (-)^m f^{(m)}(x_0),$$

valid for any function $f(x)$ which is m times differentiable at the point $x = 0$.

The main properties of the derivative of the Dirac delta function are the following:

$$\delta^{(m)}(x) = (-)^m \delta^{(m)}(-x).$$

In particular,

$$\int_{-\infty}^{+\infty} \delta'(x - x_0) f(x) dx = -f'(x_0)$$

$$\delta'(x) = -\delta'(-x)$$

$$\int \delta'(x - y) \delta(y - a) dy = \delta'(x - a)$$

$$x\delta'(x) = -\delta(x)$$

$$x^2\delta'(x) = 0$$

Integral representations of $\delta(x)$ and its derivative are:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk$$

This latter expression must be taken with a slight grain of salt. If $x = 0$, the integral is clearly infinite and $\delta(0)$ is infinite as is the Dirac δ function. However, when $x \neq 0$, the integral is simply an oscillating sinusoidal function extending to infinity in both directions. The average of the oscillating function can be assumed to vanish, and in this sense, the integral is a representation of the Dirac δ function.

The normalization $(1/2\pi)$ is chosen to be consistent with the convention for Fourier transform pairs. Thus, if

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk,$$

then,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}},$$

$$f(x) = \delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk.$$

Similarly, for the derivative of the δ function, we have:

$$\delta'(x) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} k e^{ikx} dk.$$

$\delta(x-x_0)$ may also be considered as the limit of a function which exhibits a very sharp peak about x_0 , and whose integral over all space remains constant and equal to 1. For instance,

$$\begin{aligned} \delta(x-x_0) &= \frac{1}{\pi} \lim_{L \rightarrow \infty} \sin \frac{L(x-x_0)}{x-x_0} \\ &= \frac{1}{\pi} \lim_{\kappa \rightarrow \infty} \frac{1 - \cos \kappa(x-x_0)}{\kappa(x-x_0)^2} \\ &= \frac{1}{\pi} \lim_{\epsilon \rightarrow +0} \frac{\epsilon}{(x-x_0)^2 + \epsilon^2} \\ &\lim_{\eta \rightarrow 0} \frac{\Theta(x-x_0+\eta) - \Theta(x-x_0)}{\eta} \end{aligned}$$

In the last expression, Θ is the (Heaviside) step function:

$$\Theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases}$$

(The Dirac delta function is the derivative of the step function.)

We also have an associated result,

$$\lim_{\epsilon \rightarrow +0} \frac{1}{x-x_0 \pm i\epsilon} = PP \frac{1}{x-x_0} \mp i\pi\delta(x-x_0)$$

where PP denotes the “principal part.”

Chapter 9

Almost All You Need to Know About Hermite Polynomials

The time-independent Schroedinger equation for the simple harmonic oscillator takes the form:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_n}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi_n = E_n \psi_n.$$

If we define a dimensionless variable,

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x,$$

the equation can be put into dimensionless form,

$$\frac{d^2\psi_n}{d\xi^2} + \left(\frac{2E_n}{\hbar\omega} - \xi^2\right)\psi_n = 0.$$

This equation has a known solution under the condition that

$$\frac{2E_n}{\hbar\omega} = 2n + 1,$$

i.e.,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

The solution,

$$\psi_n = AH_n e^{-\frac{\xi^2}{2}}$$

is given in terms of the so-called Hermite polynomials, H_n and an overall normalizing constant A .

Hermite polynomials are polynomials of degree n , parity $(-)^n$, having n zeros.

Rodrigues Formula:

$$H_n(\xi) = (-)^n e^{\xi^2} \left(\frac{d^n}{d\xi^n} e^{-\xi^2} \right)$$

Generating function:

$$\exp(-s^2 + 2s\xi) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi)$$

Recursion relations:

$$\begin{aligned} \frac{d}{d\xi} H_n(\xi) &= 2n H_{n-1} \\ (2\xi - \frac{d}{d\xi}) H_n(\xi) &= H_{n-1} \\ 2\xi H_n(\xi) &= H_{n+1} + 2n H_{n-1} \end{aligned}$$

Normalized solutions u_n to Schroedinger's equation for the simple harmonic oscillator:

$$u_n = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}.$$

Orthonormality:

$$\begin{aligned} \int_{-\infty}^{+\infty} u_n(\xi) u_p(\xi) d\xi &= \delta_{np} \\ \sum_{n=0}^{\infty} u_n^*(\xi) u_n(\xi') &= \delta(\xi - \xi') \end{aligned}$$

Recursion:

$$\begin{aligned} \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi} \right) u_n &= \sqrt{n} u_{n-1} \\ \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi} \right) u_n &= \sqrt{n+1} u_{n+1} \\ \xi u_n(\xi) &= \sqrt{\frac{n+1}{2}} u_{n+1} + \sqrt{\frac{n}{2}} u_{n-1} \end{aligned}$$

Parity, $(-)^n$:

$$u_n(-\xi) = (-)^n u_n(\xi)$$

Chapter 10

Almost All You Need to Know About the Hydrogen Atom Solutions

The time independent Schroedinger equation for hydrogen-like atoms is

$$\frac{1}{2m_r r^2} \left[-\hbar^2 \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \hat{L}^2 \right] \psi(r, \theta, \phi) - \frac{Ze^2}{4\pi\epsilon_0 r} \psi(r, \theta, \phi) = E\psi(r, \theta, \phi),$$

where e is the charge on the electron, Ze is the charge on the nucleus, and m_r is the reduced mass of the system,

$$m_r = \frac{m_e M}{m_e + M} \approx m_e.$$

The mass of the electron is m_e and the mass of the nucleus is M . The differential operators \hat{L}^2 and \hat{L}_z derive from the angular momentum operator,

$$\hat{\mathbf{L}} = -i\hbar \mathbf{r} \times \nabla.$$

They are,

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right],$$
$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

Schroedinger's Equation can be solved by separation of variables,

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) = ru(r)Y(\theta, \phi).$$

10.1 Angular Equation

The solutions $Y(r, \theta, \phi)$ to the angular equation are simultaneous eigenfunctions of \hat{L}^2 and \hat{L}_z ,

$$\hat{L}^2 Y_\ell^m(\theta, \phi) = \hbar^2 \ell(\ell + 1) Y_\ell^m(\theta, \phi),$$

$$\hat{L}_z Y_\ell^m(\theta, \phi) = m \hbar Y_\ell^m(\theta, \phi).$$

The functions $Y_\ell^m(\theta, \phi)$ are called *Spherical Harmonic Functions* and they are built up in the following way.

Solutions to the differential equation,

$$\frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + [\ell(\ell + 1) \sin \theta] \Theta = 0$$

are the *Legendre Polynomials*,

$$\Theta(\theta) = A P_\ell(\cos \theta)$$

generated by the Rodrigues formula,

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx} \right)^\ell (x^2 - 1)^\ell.$$

Legendre polynomials satisfy the normalization condition,

$$\int_{-1}^{+1} P_\ell(x) P_{\ell'}(x) dx = \int_0^\pi P_\ell(\cos \theta) P_{\ell'}(\cos \theta) \sin \theta d\theta = \frac{2}{2\ell + 1} \delta_{\ell\ell'}.$$

Associated Legendre Polynomials $\Theta = A P_\ell^m(\cos \theta)$ are solutions to

$$\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + [\ell(\ell + 1) \sin^2 \theta - m^2] \Theta = 0$$

and are generated from

$$P_\ell^m(x) = (1 - x^2)^{|m|/2} \left(\frac{d}{dx} \right)^{|m|} P_\ell(x).$$

Associated Legendre polynomials satisfy the normalization condition,

$$\int_{-1}^{+1} P_\ell^m(x) P_{\ell'}^m(x) dx = \left(\ell + \frac{1}{2} \right)^{-1} \frac{(\ell + m)!}{(\ell - m)!} \delta_{\ell\ell'}$$

Spherical Harmonic Functions $Y_\ell^m(\theta, \phi)$ are solutions (obtained by separation of variables) to

$$\sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) Y(\theta, \phi) + [\ell(\ell + 1) \sin^2 \theta] Y(\theta, \phi) + \frac{\partial^2}{\partial \phi^2} Y(\theta, \phi) = 0.$$

The spherical harmonics are derived from the associated Legendre polynomials,

$$Y_\ell^m(\theta, \phi) = A P_\ell^m(\theta) e^{im\phi}.$$

These are normalized to unity,

$$\int_0^{2\pi} \int_0^\pi [Y_\ell^m(\theta, \phi)]^* [Y_{\ell'}^{m'}(\theta, \phi)] \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'},$$

by choosing the normalization constant A to be

$$A = \epsilon \sqrt{\frac{2(\ell + 1)(\ell - |m|)!}{4\pi(\ell + |m|)!}}$$

$$\epsilon = (-1)^m, \quad m \geq 0$$

$$\epsilon = 1, \quad m < 0.$$

10.2 Radial Equation

Solutions to Schroedinger's Equation obtained by separation of variables thus become,

$$\psi(r, \theta, \phi) = R(r) Y_\ell^m(\theta, \phi).$$

The radial equation becomes,

$$\frac{1}{2m_r r^2} \left[-\hbar^2 \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \hbar^2 \ell(\ell + 1) \right] R(r) - \frac{Ze^2}{4\pi\epsilon_0 r} R(r) = ER(r).$$

Defining and substituting,

$$\kappa = -\frac{2m_r E}{\hbar^2}, \quad \rho = \kappa r, \quad \rho_0 = \frac{m_r Z e^2}{2\pi\epsilon_0 \hbar^2 \kappa}$$

and,

$$R(r) = \frac{u(r)}{r},$$

we obtain,

$$\frac{d^2}{d\rho^2}u(\rho) - \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]u(\rho) = 0.$$

Solutions to this equation are of the form,

$$u(\rho) = \rho^{\ell+1}e^{-\rho}v_{n\ell}(\rho),$$

where,

$$v_{n\ell}(\rho) = L_{n-\ell-1}^{2\ell+1}, \quad n = 1, 2, 3, \dots; \ell = 0, \dots, n-1$$

are the *Associated Laguerre Polynomials* generated from,

$$L_{q-p}^p(x) = (-1)^p \left(\frac{d}{dx}\right)^p L_q(x)$$

and $L_q(x)$ are the *Laguerre Polynomials* generated from

$$L_q(x) = e^x \left(\frac{d}{dx}\right)^q (e^{-x}x^q).$$

10.3 Summary

Summarizing, normalized solutions to Schroedinger's equation for hydrogen-like atoms are:

$$\psi_{n\ell m} = \sqrt{\left(\frac{2Z}{na'_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+1)!]^3}} e^{-Zr/na'_0} \left(\frac{2Zr}{na'_0}\right)^\ell [L_{n-\ell-1}^{2\ell+1}(2Zr/na'_0)] Y_\ell^m(\theta, \phi),$$

$$\int \psi_{n\ell m}^* \psi_{n'\ell'm'} r^2 \sin\theta dr d\theta d\phi = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'},$$

where the reduced mass m_r is given by

$$m_r = \frac{m_e M}{(m_e + M)} = \frac{m_e}{(1 + m_e/M)} \approx m_e,$$

the Bohr radius is,

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2},$$

the Bohr radius corrected for the reduced mass is,

$$a'_0 = a_0(1 + m_e/M)$$

and the energy eigenvalues are,

$$E_n = -\frac{m_r Z^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} = -\frac{1}{2} \alpha^2 (m_e c^2) \left(1 + \frac{m_e}{M}\right)^{-1} \frac{Z^2}{n^2}.$$

the charge on the electron is e , the charge on the nucleus is Ze , the mass of the electron is m_e , the mass of the nucleus is M and the fine structure constant is α .

$$E_0 = -\frac{1}{2} \alpha^2 (m_e c^2) = -13.6 \text{ eV}.$$

The integer n takes the values $n = 1, 2, \dots, \infty$. The integer ℓ takes values $\ell = 0, \dots, n - 1$ and the index m take values $m = -\ell, -\ell + 1, \dots, \ell - 1, \ell$.

Chapter 11

Almost All You Need to Know About Fourier Transforms

The *Fourier transform* of $f(x)$ is the function $F(k)$ defined by,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx.$$

The *inverse Fourier transform* of $F(k)$ is defined by,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{+ikx} dk.$$

Table of Fourier Transforms

$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k)e^{+ikx} dk$	$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)e^{-ikx} dx$
$f\left(\frac{x}{c}\right)$	$ c F(ck)$
$f(-x)$	$F(-k)$
$f^*(x)$	$F^*(-k)$
$xf(x)$	$iF'(k)$
$f'(x)$	$ikF(k)$
$f(x - x_0)$	$e^{-ikx_0}F(k)$
$e^{ik_0x}f(x)$	$F(k - k_0)$
$\delta(x)$	$\left(\frac{1}{2\pi}\right)^{\frac{1}{2}}$
$\delta(x - x_0)$	$\left(\frac{1}{2\pi}\right)^{\frac{1}{2}}e^{-ikx_0}$
$\left(\frac{\kappa}{\sqrt{\pi}}\right)^{\frac{1}{2}}e^{-\frac{1}{2}\kappa^2x^2}$	$\left(\frac{1}{\kappa\sqrt{\pi}}\right)^{\frac{1}{2}}e^{-k^2/2\kappa^2}, \text{ Re } \kappa > 0, \text{ Re } \kappa^2 > 0$
$\Theta(x)$, step function	$\frac{1}{\sqrt{2\pi}}[\pi\delta(k) - iPP\frac{1}{k}]$