Graduate Quantum Mechanics

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Acknowledgements

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Chapter 1

Mathematical Background

"Our description of the physical world is dynamic in nature and undergoes frequent change. At any given time, we summarize our knowledge of natural phenomena by means of certain laws. These laws adequately describe the phenomenon studied up to that time, to an accuracy then attainable. As time passes, we enlarge the domain of observation and improve the accuracy of measurement. As we do so, we constantly check to see if the laws continue to be valid. Those laws that do remain valid gain in stature, and those that do not must be abandoned in favor of new ones that do." - R. Shankar

In classical mechanics, we learned how objects interact with each other and move around and so on. However, this formulation starts to fall apart as we make those objects smaller and smaller. Quantum mechanics deals with the nature of atomic and subatomic particles. Before we begin though, we should introduce some mathematical background and language that makes this subject a little more manageable.

1.1 Bra-Ket Notation

In your introductory physics classes, you were introduced to vectors as arrows which have a magnitude and a direction. In this section, we'll introduce a new way of looking at vectors that does away with the arrows. It may seem that we're getting rid of the fundamental nature of vectors, but we're really just expanding our definition of what a vector is.

1.1.1 Ket Space

In undergraduate physics (and most of the other graduate physics), we refer to a vector as $\vec{x}$. In quantum mechanics, we instead use bra-ket notation, developed by Dirac. The vector $\vec{x}$ is now written as $|x\rangle$. For now, it might be helpful to think of vectors using the old arrow system.

There is a whole discussion about vector spaces that we won't get into here. For more information, you should be able to find this in just about any quantum physics textbook. Our ket $\vec{x}$ contains complete information about a physical state, which is represented by a state vector in complex vector space.

1.1.2 Bra Space

Just as we have ket space, we have bra space, the dual of ket space. If our ket can be written as a column vector, then the bra is the row vector that is the complex conjugate transpose of that ket. Furthermore, we note that the dual of a scalar multiplied by a ket is not a scalar multiplied by a bra, but rather the complex conjugate of the scalar multiplied by the bra, i.e., the dual is given by equation (1.1).

$$c_\alpha |\alpha\rangle + c_\beta |\beta\rangle \leftrightarrow c_\alpha^* \langle\alpha| + c_\beta^* \langle\beta| \tag{1.1}$$

Now that we have both bra and ket spaces, we can define an inner product, or scalar product (1.2). This works in much the same way as the scalar product that you are used to from undergrad. If we take the inner product of two vectors and get 0, we say the two vectors are orthogonal (1.3). We can define the length, or norm, of a vector as the square root of the inner product (1.4).

$$\langle\alpha|\beta\rangle \tag{1.2}$$

$$\langle\alpha|\beta\rangle = 0 \tag{1.3}$$

$$|V| = \sqrt{\langle V|V\rangle} \tag{1.4}$$

We state here two theorems: the Schwarz Inequality (1.5) and the Triangle Inequality (1.6)

$$|\langle V|W\rangle| \leq |V||W| \tag{1.5}$$

$$|V + W| \leq |V| + |W| \tag{1.6}$$

1.1.3 Linear Independence

Every vector-space has some dimension which is equal to the number of linearly independent basis vectors. Going back to our example of a ket as a column vector, the dimension would be equal to the number of entries in that vector. In any given vector space, we can write any vector in that space as a linear combination of n linearly independent vectors, $|i\rangle$ (1.7). We know these vectors are linearly independent if the only way to write the null vector is by setting all v_i equal to 0, the trivial case.

$$|V\rangle = \sum_{i=1}^{n} v_i |i\rangle \tag{1.7}$$

1.1.4 Gram-Schmidt Theorem

Let's say we have our linearly independent basis. We now want to make that basis orthonormal. We want it to be orthogonal so we can write our vector easily as a combination of the basis vectors. We want there to be only one way to write that vector. We want it to be normal (length of unity) because, as we shall see, the probability of a particle being in a certain state can be found by taking an inner product.

To take some linearly independent basis into an orthonormal one, we use the Gram-Schmidt procedure. We take the first basis vector and normalize it. We then take the second vector,

$$|2'\rangle = |II\rangle - |1\rangle \langle 1|II\rangle$$

where $|2'\rangle$ is the unnormalized, orthogonal second basis vector, $|1\rangle$ is the normalized first basis vector, and $|II\rangle$ is the original second basis vector. We then normalize to get our second basis vector. For the third vector,

$$|3'\rangle = |III\rangle - |1\rangle \langle 1|III\rangle - |2\rangle \langle 2|III\rangle$$

We continue in this manner until we have all of our orthonormal basis vectors.

1.1.5 Example: Spin-$1/2$ Systems

In spin-$1/2$, we have a two-dimensional system represented by the basis kets, $|+\rangle$ and $|-\rangle$. We generally represent these using the vectors,

$$\begin{cases} |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \\ |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{cases}$$

We can easily convince ourselves that this forms an orthonormal basis. If we have a particle floating along with no bias towards either state, we represent it,

$$|\Psi\rangle = 1/\sqrt{2}(|+\rangle + |-\rangle)$$

It can be either spin-up or spin-down, and we won't know until we make a measurement.

You should now be able to do Shankar 1.1.1, 1.1.2, 1.1.3, 1.1.4, 1.1.5, 1.3.1, 1.3.2, 1.3.3, 1.3.4, 1.4.1, and 1.4.2.

1.2 Operators

An operator is a sort of instruction for transforming a vector $|V\rangle$ to another vector $|V'\rangle$ (1.8). In this section, we will discuss properties of operators as well as define some terms. Just as we thought of kets as column matrices and bras as row matrices, we can think of operators as square matrices. Going forward, this is probably the easiest way to visualize them.

$$\Omega\,|V\rangle = |V'\rangle \tag{1.8}$$

As an example, let's say we want an operator that rotates a vector by $\pi/2$ about the $\hat{i}$ axis. We call this operator, $R(\pi/2\ \hat{i})$. When we act this operator on the basis vectors, we want it to have the following effect,

$$\begin{cases} R(\pi/2\ \hat{i})\,|i\rangle = |i\rangle \\ R(\pi/2\ \hat{i})\,|j\rangle = |k\rangle \\ R(\pi/2\ \hat{i})\,|k\rangle = -\,|j\rangle \end{cases}$$

If we write the basis kets in the usual vector notation, i.e., $|i\rangle = (1, 0, 0)$ and so on, we can see the matrix representation of our operator is

$$R(\pi/2\ \hat{i}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

1.2.1 Definitions

From linear algebra, we remember that in general, $AB \neq BA$ where A and B are matrices. The same is true for operators, i.e., the order of operators is important. To this end, we define the commutator of two operators Ω and Λ using equation (1.9). If the commutator of two operators is zero, we say those two operators commute. We also define the anti-commutator using equation (1.10).

$$[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega \tag{1.9}$$

$$\{\Omega, \Lambda\} = \Omega\Lambda + \Lambda\Omega \tag{1.10}$$

The inverse of matrix Ω is denoted Ω^{-1} and satisfies equation (1.11). Note that an operator commutes with its inverse. Further note that not every operator has an inverse. The inverse of a product of operators must follow equation (1.12).

$$\Omega\Omega^{-1} = \Omega^{-1}\Omega = I \tag{1.11}$$

$$(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1} \tag{1.12}$$

We also want to define Hermitian (1.13) and Unitary operators (1.14). We define the † symbol to mean the adjoint, which means to take the transpose conjugate of the original operator.

$$\Omega^{\dagger} = \Omega \tag{1.13}$$

$$\Omega\Omega^{\dagger} = \Omega^{\dagger}\Omega = I \tag{1.14}$$

The adjoint of a product of operators (1.15) follows the same rule as the inverse.

$$(\Omega\Lambda)^{\dagger} = \Lambda^{\dagger}\Omega^{\dagger} \tag{1.15}$$

1.2.2 Projection Operator

One special operator we should mention is the projection operator (1.16). Imagine we have our base kets and we want to find the portion of a ket that is parallel to a specific base kets. This is useful for finding the coefficients in equation (1.7). If we sum over all the projection operators, we get the completeness relation (1.17). This is what we insert into a chain of bras and kets when we insert the identity operator.

$$\Lambda_{a'} = |a'\rangle \langle a'| \tag{1.16}$$

$$\sum_{a'} \Lambda_{a'} = \sum_{a'} |a'\rangle \langle a'| = 1 \tag{1.17}$$

One property of projection operators is that if the kets are normalized, then $\Lambda_{a'}^2 = \Lambda_{a'}$. We can show this by writing it out explicitly,

$$\Lambda_{a'}^2 = \Lambda_{a'} \Lambda_{a'}^*$$

$$= |a'\rangle \langle a'|a'\rangle \langle a'|$$

Since the kets are normalized, the middle part disappears and we are left with the original projection operator. Alternatively, we can think about this logically. If we apply multiple projection operators (multiple of the same projection operator) onto a vector, nothing should happen after the first projection operator.

1.2.3 Matrix Elements of Operators

Let's say we have specified the base kets and we want to now write an operator in that basis. We start with our operator and multiply by an identity matrix on both sides,

$$\Omega = \sum_{a''} \sum_{a'} |a''\rangle \langle a''|\Omega|a'\rangle \langle a'|$$

The middle component is just a scalar and the left and right components give the position of that matrix element, i.e.,

$$\Omega = \begin{bmatrix} \langle a^{(1)}|\Omega|a^{(1)}\rangle & \langle a^{(1)}|\Omega|a^{(2)}\rangle & ... \\ \langle a^{(2)}|\Omega|a^{(1)}\rangle & \langle a^{(2)}|\Omega|a^{(2)}\rangle & ... \\ \vdots & \vdots & \ddots \end{bmatrix}$$

As an example, let's look at the rotation matrix, which we'll simplify as R_x.

$$R_x = \begin{bmatrix} \langle i|R_x|i\rangle & \langle i|R_x|j\rangle & \langle i|R_x|k\rangle \\ \langle j|R_x|i\rangle & \langle j|R_x|j\rangle & \langle j|R_x|k\rangle \\ \langle k|R_x|i\rangle & \langle k|R_x|j\rangle & \langle k|R_x|k\rangle \end{bmatrix}$$

Using the formulation from before,

$$= \begin{bmatrix} \langle i|i\rangle & \langle i|k\rangle & \langle i| - j\rangle \\ \langle j|i\rangle & \langle j|k\rangle & \langle j| - j\rangle \\ \langle k|i\rangle & \langle k|k\rangle & \langle k| - j\rangle \end{bmatrix}$$

Since the basis vectors are orthonormal,

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

You should now be able to do Shankar 1.6.1, 1.6.2, 1.6.3, 1.6.4, 1.6.5, 1.6.6, 1.7.1, and 1.7.2.
You should now be able to do Sakurai 1.1, 1.2, 1.3, 1.4, 1.5, and 1.8.
You should now be able to do Cohen-Tannoudji 2.3, 2.4, 2.5, and 2.6.

1.3 Eigenvalues

And now we get into the real meat of quantum mechanics. Imagine we act our operator on any ket, we can imagine that there are some special cases where the action simply re-scales the vector. These special kets are known as the eigenkets (or eigenvectors) of an operator, and the value by which they are re-scaled are the eigenvalues. Quick note, those of you who know German will recognize that *eigen* means *same* in German. As Shankar put it, "once we get to quantum mechanics proper, it will be eigen, eigen, eigen all the way."

1.3.1 The Characteristic Equation

There are some number of operators that we can find the eigenkets just by thinking. For example, a rotation about the x-axis. If we have a vector along the x-axis, then rotation won't change it. But there are many other operators that we can't just think about and solve. For those, we have a specific equation to solve (1.18) where $|V\rangle$ is the eigenket and ω is the eigenvalue.

$$\Omega |V\rangle = \omega |V\rangle \tag{1.18}$$

Rearranging,

$$(\Omega - \omega I) |V\rangle = |0\rangle$$

Taking the determinant of both sides,

$$\det(\Omega - \omega I) = 0 \tag{1.19}$$

Solving, we get the solution,

$$\sum_{m=0}^{n} c_m \omega^m = 0 \tag{1.20}$$

Equation (1.20) is referred to as the characteristic equation where the roots are the eigenvalues. Once we know the eigenvalues, we should be able to substitute them back in and solve for the eigenkets.

Before, we mentioned Hermitian operators (1.13). We like Hermitian operators in quantum mechanics because they have certain properties. First, the eigenvalues of a Hermitian operator are real. Second, for every Hermitian operator, there exists a basis consisting of its orthonormal eigenvectors. We can create a unitary matrix U built out of the eigenvectors of Ω such that $U^\dagger \Omega U$ is diagonal. What this means if if we want a basis that diagonalizes Ω, we just need to solve the eigenvalue problem.

We have similar rules for unitary operators. The eigenvalues of a unitary operator are complex numbers of unit modulus. The eigenvectors of a unitary operator are mutually orthogonal.

1.3.2 Example: Eigenvalues of Rotation around x-axis

As an example, let's find the eigenkets of a rotation around the x-axis by $\pi/2$. We already know one eigenvalue from thinking about it, but are there more? As a reminder,

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

Let's now get the characteristic equation (1.20),

$$\det(R_x - \omega I) = \det \begin{bmatrix} 1-\omega & 0 & 0 \\ 0 & -\omega & -1 \\ 0 & 1 & -\omega \end{bmatrix} = 0$$

$$(1-\omega)(\omega^2+1) = 0$$

The roots are $\omega = 1, \pm i$, so those are the eigenvalues. The corresponding eigenkets, we label $|1\rangle, |i\rangle, |-i\rangle$. We'll start with $|1\rangle$. We expect this to be a vector lying in the x-axis,

$$(R_x - I)|1\rangle = |0\rangle$$

$$\begin{bmatrix} 1-1 & 0 & 0 \\ 0 & 0-1 & -1 \\ 0 & 1 & 0-1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{cases} 0 = 0 \\ -b - c = 0 \\ b - c = 0 \end{cases}$$

We have constraints on b and c ($b = c = 0$), a can be whatever we want, so let's normalize it,

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Let's move on to $|i\rangle$,

$$(R_x - iI)|i\rangle = |0\rangle$$

$$\begin{bmatrix} 1-i & 0 & 0 \\ 0 & 0-i & -1 \\ 0 & 1 & 0-i \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{cases} (1-i)a = 0 \\ -ib - c = 0 \\ b - ic = 0 \end{cases}$$

$$|i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ i \\ 1 \end{bmatrix}$$

Similarly,

$$|-i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix}$$

1.3.3 Example: Degenerate Hermitian Matrix

Imagine we have Hermitian matrix,

$$\Omega = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

Solving the characteristic equation (1.20),

$$\det(\Omega - \omega I) = \det \begin{bmatrix} 1-\omega & 0 & 1 \\ 0 & 2-\omega & 0 \\ 1 & 0 & 1-\omega \end{bmatrix} = 0$$

$$(1-\omega)^2(2-\omega) - 0 + 1(-1)(2-\omega) = 0$$

$$= (\omega - 2)(\omega^2 - 2\omega)$$

$$\omega(\omega - 2)^2 = 0$$

Unfortunately, we have a degeneracy, i.e., repeated eigenvalues, $\omega = 0, 2, 2$. One of these is not degenerate, so let's find that eigenket,

$$(\Omega)\,|0\rangle = 0$$

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{cases} a + c = 0 \\ 2b = 0 \end{cases}$$

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Event though we have a degeneracy, we can still find one eigenket for that eigenvalue,

$$(\Omega - 2I)\,|2_1\rangle = 0$$

$$\begin{bmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{cases} -a + c = 0 \\ b \ arbitrary \end{cases}$$

$$|2_1\rangle = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

We note the second term is arbitrary. Using this in conjunction with orthonormalizing the eigenkets, we can actually get a second eigenket for $\omega = 2$,

$$|2_2\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

We now have an orthonormal set of eigenkets. We can diagonalize Ω by creating the unitary matrix from the eigenkets,

$$U = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{3} & 1/\sqrt{6} \\ 0 & 1/\sqrt{3} & -2/\sqrt{6} \\ -1/\sqrt{2} & 1/\sqrt{3} & 1/\sqrt{6} \end{bmatrix}$$

To prove that this diagonalizes Ω, we use brute force,

$$U^\dagger \Omega U = \begin{bmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{6} & -2/\sqrt{6} & 1/\sqrt{6} \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{3} & 1/\sqrt{6} \\ 0 & 1/\sqrt{3} & -2/\sqrt{6} \\ -1/\sqrt{2} & 1/\sqrt{3} & 1/\sqrt{6} \end{bmatrix}$$

$$= \begin{bmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{6} & -2/\sqrt{6} & 1/\sqrt{6} \end{bmatrix} \begin{bmatrix} 0 & 2/\sqrt{3} & 2/\sqrt{6} \\ 0 & 2/\sqrt{3} & -4/\sqrt{6} \\ 0 & 2/\sqrt{3} & 2/\sqrt{6} \end{bmatrix}$$

$$U^\dagger \Omega U = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

We get a diagonal matrix whose elements are the eigenvalues.

1.3.4 Simultaneous Diagonalization

If we have two commuting Hermitian operators, A and B, we can find a basis of common eigenvectors that diagonalizes both. We can have a Complete Set of Commuting Observables (CSCO) if every observable in the set commute with every other observable in that set and if specifying all the eigenvalues determines a unique common eigenvector. That is, if we list each common eigenvector for each observable, no two eigenvectors should have the same eigenvalues for every observable.

You should now be able to do Shankar 1.8.1, 1.8.2, 1.8.3, 1.8.4, 1.8.5, 1.8.6, 1.8.7, 1.8.8, 1.8.9, and 1.8.10.

You should now be able to do Sakurai 1.6, 1.7, 1.9, 1.10, 1.11, 1.14, 1.15, 1.16, 1.17, 1.23, and 1.24.

You should now be able to do Cohen-Tannoudji 2.1, 2.2, 2.7, 2.11, and 2.12.

1.4 Functions of Operators

It is useful to know what happens when we take the function of some operator. We will consider only those functions that can be written as power series,

$$f(x) = \sum_{n=0}^{\infty} a_n x^n$$

1.4.1 Converging Sums

We can define the function of an operator in much the same way (1.21).

$$f(\Omega) = \sum_{n=0}^{\infty} a_n \Omega^n \tag{1.21}$$

1.4.2 Derivatives

Derivatives are taken normally.

You should now be able to do Shankar 1.9.1, 1.9.2, 1.9.3, 1.10.1, 1.10.2, and 1.10.3.