Graduate Quantum Mechanics

Benjamin D. Suh

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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 phenomenon 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 stature, and those that do not must be abandoned in favour 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 more manageable.

1.1 Vector Spaces and 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 courses in graduate school), 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 $|x\rangle$. It might be helpful to think of vectors using the old arrow system, but we will to eventually start distancing ourselves from that implementation. Imagine we have a collection of vectors. These vectors form a linear vector space if they follow a set of rules laid out in any quantum textbook.

1.1.2 Bra Space

Just as we have ket space, bra space is the dual of ket space. Imagine that our ket represents a row vector. In this case, our bra represents a column vector with all of the elements having been complex conjugated. 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, $c^* \langle\alpha|$. If we multiply a bra by a ket, we get an inner product (1.1), which is a scalar. If we take the inner product of two vectors and we get 0, we say the two vectors are orthogonal. We define the length, or norm (1.2), of a vector as the square root of the inner product.

$$\langle\alpha|\beta\rangle \tag{1.1}$$

$$|V| = \sqrt{\langle V|V\rangle} \tag{1.2}$$

1.1.3 Linear Independence

Every vector-space has some dimension, which is equal to the number of linearly independent basis vectors (1.3). That is, in any given vector space, we can write any vector in that space as a linear combination of n linearly independent vectors, $|i\rangle$. We know that 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.

$$|V\rangle = \sum_{i=1}^{n} v_i |i\rangle \tag{1.3}$$

1.1.4 Gram-Schmidt Theorem

Let's say we have our linearly independent basis. We now want to make that basis orthonormal. To do this, we use the following procedure. First, we take the first basis vector and normalize it. We then take the second vector and perform

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

We can 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 then continue until we have all of our orthonormal basis vectors.

1.1.5 Example: Stern-Gerlach Experiment

In spin-1/2 systems, we have a two-dimensional system. Our basis vectors are

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

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

We can easily convince ourselves that this forms an orthonormal basis.

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 an instruction for transforming a vector (1.4). In this section, we will discuss properties of operators as well as define some terms.

$$\Omega \left| V \right\rangle = \left| V' \right\rangle \tag{1.4}$$

As an example, let's say we want an operator that rotates a vector by $\pi/2$ around the $\hat{i}$ axis. We'll call this operator, $R\left(\frac{\pi}{2}\hat{i}\right)$. Thinking about it, when we act this operator on the basis vectors,

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

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

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

Go ahead and check that is true.

1.2.1 Definitions

From linear algebra, we remember that $AB \neq BA$ 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 (1.5). If the commutator of two operators is zero, we say those two operators commute.

$$\Omega\Lambda - \Lambda\Omega = [\Omega, \Lambda] \tag{1.5}$$

The inverse of matrix Ω is denoted Ω^{-1} and satisfies equation 1.6. You may note that an operator commutes with its inverse. Note that not every operator has an inverse. Further, the inverse of a product of operators must follow equation (1.7).

$$\Omega\Omega^{-1} = \Omega^{-1}\Omega = I \tag{1.6}$$

$$(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1} \tag{1.7}$$

We also want to define Hermitian (1.8) and Unitary operators (1.9). We define the † symbol to mean the adjoint. We take the transpose conjugate of the original operator.

$$\Omega^{\dagger} = \Omega \tag{1.8}$$

$$\Omega\Omega^{\dagger} = \Omega^{\dagger}\Omega = I \tag{1.9}$$

1.2.2 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 identity on both sides,

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

The middle section gives us the matrix elements, i.e.,

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

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

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

Since the basis vectors are orthonormal,

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

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

1.3.1 Characteristic Equation and Determining Eigenvalues

1.3.2 Eigenkets

1.3.3 Degeneracy

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, 1.12, 1.13, 1.14, 1.15, 1.16, 1.17, 1.18, 1.19, 1.20, 1.21, 1.22, 1.23, 1.24, 1.25, 1.26, 1.27, 1.28, 1.29, 1.30, 1.31, 1.32, and 1.33.

You should now be able to do Cohen-Tannoudji 2.1, 2.2, 2.7, 2.8, 2.9, 2.10, 2.11, and 2.12.