

# Why Quantum Mechanics is (mostly) Obvious

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## Abstract

The mathematical techniques used in quantum mechanics are applied to simple examples of random variables. This illustrates many of the mathematical features of quantum mechanics without confusing them with the physical content of the theory. The mathematical postulates of quantum mechanics can then be presented as plausible extensions of these ideas.

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A first course in quantum mechanics (QM) can seem conceptually difficult at first. There are two principle obstacles. The first is the new physics involved: the photon nature of light, the wave nature of electrons, the uncertainty principle, the quantisation of energy levels and so on. The second obstacle is the mathematical framework used by quantum mechanics: vector spaces, state vectors, commutators, probability amplitudes and so on, as fully outlined by Dirac [1]. It is easy to confuse these two aspects of QM and come to view them as inseparable. This paper applies the mathematical methods of QM to a series of simple examples and so helps to isolate the mathematics from the physics.

The style is intentionally informal and certainly not rigorous. It is not intended to be a course on QM. Rather, it is intended as supplementary material that helps to make the postulates of QM seem more plausible. In a typical QM course it might be introduced just after outlining the need for QM but before listing the postulates themselves.

## 1. Summary of Probability Theory and Linear Algebra

The amount of probability theory we require is minimal and will be illustrated with examples. A more detailed coverage of probability and statistics is available in a host of introductory texts, such as Boas [2] or MIT [10].

Suppose we take an ordinary six sided die. Assuming the die is fair, when we throw the die we would expect an equal probability of any particular side landing face up. So if we throw the die 60 times, we would expect, roughly, 10 outcomes to correspond to each side of the die, perhaps a few more for some and a few less for others. As we steadily increase the number of throws, we expect the proportion of throws corresponding to each face of the die to approach  $1/6$ . We say that the probability of measuring each particular value is  $1/6$ .

In terms of notation, if  $d$  is the value of the die that lands face up, then we write:

$$P(d = i) = 1/6, \quad i=1,2,3,4,5,6$$

We read this as “*the probability that  $d = i$  is  $1/6$* ”.

The probability of a particular outcome does not always have to be the same as all other possible outcomes. Continuing with the example of the die, suppose we are interested in values where  $d > 2$ . There are four ways that this could happen: 3,4,5,6, out of the six possible die values. So

$$P(d > 2) = 4/6 = 2/3,$$
$$P(d \leq 2) = 2/6 = 1/3.$$

Notice that, as in the case of our first die example, the total probability of all possible outcomes is always one: at least one of the outcomes is certain to happen. This is an example of a **probability distribution**. It is the set of all probabilities for all possible outcomes. It's values always add up to one.<sup>1</sup>

The value of the die that lands face up is an example of a **random variable**. Anything that can be measured can be regarded as a random variable, even something that we think we know with absolute certainty. An absolutely certain outcome is simply a measurement of a random variable with a probability of one. A completely impossible outcome has a probability of zero. So when we state that a measurement is made of a “random” variable, we are not prejudicing our assumptions: random does not mean equally likely, and could mean certain or impossible or anything in between. It all depends on the probability distribution.

Sometimes the probability of a particular outcome depends on the conditions. For example, we can write  $P(d = 2) = 1/6$ . This assumes that all values of the die are equally likely. Now suppose someone else throws the die and then hides the value from us. They do tell us that the value is even, however. The probability of the die showing 2 is now quite different. There are only three even values. In this case we write:

$$P(d = 2 \mid d \text{ is even}) = 1/3.$$

This should be read as “*the probability that  $d$  is 2, given that we know  $d$  is even, is  $1/3$* .” We will find that almost all probability calculations in QM are conditional probability calculations.

That is all the probability theory that we need to know for the examples in this paper. Next we have a brief look at vector spaces and linear algebra. This is necessarily a minimalist overview of the subject. For more comprehensive coverage see any good introductory text on quantum mechanics, such as Binney and Skinner [3] or Griffiths [4] or Shankar [6].

I will assume that you are already familiar with the concept of **vectors** in either 2D or 3D space. You may even be familiar with 4D vectors in Minkowski space. A **vector space** is just a mathematical generalisation where any fixed size set of numbers behaves like the components of geometrical vectors. The fixed size can be any positive integer and is called the **dimension** of the vector space.

We can write any vector as a row or as a column, listing its components. e.g. In a 5 dimensional vector space we might have a row vector (1, 2, 3.14, 2.72, -1). We can add two row vectors or two column vectors just by adding their components. We can multiply a vector by a number simply by multiplying all of its components.

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<sup>1</sup> The notion that all the probabilities in a distribution add up to one is a convention, but it is a convention that is so useful and so universally adopted that there is no reason to deviate from it.

Any vector can be written as a sum of its components times the corresponding **basis vectors**. Basis vectors are just unit length vectors along each dimension of the vector space. e.g. The above row vector can be written:

$$(1, 2, 3.14, 2.72, -1) =$$

$$\begin{aligned} & 1 \quad \times (1,0,0,0,0) + \\ & 2 \quad \times (0,1,0,0,0) + \\ & 3.14 \quad \times (0,0,1,0,0) + \\ & 2.72 \quad \times (0,0,0,1,0) - \\ & 1 \quad \times (0,0,0,0,1). \end{aligned}$$

If we call the components of a vector  $v^i$  and the basis vectors  $e_i$ , then the vector  $v$  can be written as:

$$v = \sum_i v^i e_i \quad . \quad (1)$$

Suppose we have a function  $L$  that acts on a vector  $v$  and results in a new vector  $w$  in the the same vector space.  $L$  is defined to be a **linear function** if:

$$w = L(v) = \sum_i v^i L(e_i) \quad . \quad (2)$$

i.e. The function  $L$  slides past the component values and acts directly on each of the basis vectors.

As  $w$  is a vector, it has components  $w_j$ .

$$w_j = \sum_i v^i [L(e_i)]_j = \sum_i W_{ji} v^i \quad . \quad (3)$$

Where  $W_{ji}$  is the  $j$ 'th component of the action of  $L$  on the basis vector  $e_i$ .

This final expression is just the rule for multiplying the matrix  $W$  into the vector  $v$ . The bottom line of all this is that *we can always represent a linear function on a finite dimensional vector space by a matrix*. With this rule at our disposal we are now ready to look at some examples.

## 2. The Six Sided Die

Let's return to our six sided die. In this case, the act of measurement means throwing the die on a table and observing the value that eventually appears face up. To model the die we're going to use a six dimensional vector space. This six dimensional vector space has six basis vectors:  $e_1, \dots, e_6$ . Each basis vector corresponds to one value of the die. So if the value 1 is face up then the state of the die is represented by

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \quad (4)$$

If the value 2 is face up then the state of the die is represented by

$$e_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \quad (5)$$

Similarly, each of the possible measurement values 1 through 6 is represented by the basis vectors  $e_1$  through  $e_6$ . Each basis vector points entirely along one axis of the six dimensional space. The  $e_1$  vector points entirely along the “one’ness” direction, with no components in the “two’ness” or “three’ness” etc. directions. Similarly, the  $e_i$  basis vector points entirely along the  $i$ ’th direction.

Next we’re going to invent a **measurement operator** for the die. Call it  $D$ . (Operators will be shown in capital bold typeface.) This has all the possible measurement values on the diagonal and zero everywhere else.

$$D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 \end{bmatrix} \quad (6)$$

Using ordinary matrix multiplication, the operator  $D$  can act on any of the basis vectors to produce the measured value corresponding to that vector times the same vector again. For example:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 3 \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} . \quad (7)$$

And in general:

$$D e_n = n e_n . \quad (8)$$

An equation like this is called an **eigenvalue equation**. The number  $n$  is called the **eigenvalue** and the vector  $e_n$  is called the **eigenvector**. Note that if  $e_n$  is an eigenvector with eigenvalue  $n$ , then any multiple of  $e_n$ , such as  $3e_n$ , is also an eigenvector with the same eigenvalue. These are all treated as the same eigenvector.

The eigenvectors form a **complete set**. This means that any vector can be expressed as a linear combination of the eigenvectors.

Somewhere near the start of every quantum mechanics textbook, there is a list of postulates that all of quantum mechanics is based on. One of these will say something like this.

*An observable in quantum mechanics is represented by a measurement operator. The possible outcomes of a measurement are the eigenvalues of the measurement operator and the allowed states of the system when a measurement has taken place are the corresponding eigenvectors.*

This statement can seem puzzling if you haven't encountered this aspect of linear algebra before. But as you can see from the simple example of the die, it's really very straightforward.

In the case of the die, we deliberately constructed the measurement operator to be a diagonal matrix with eigenvectors that had only a single component. This is not always the case, as we will see shortly.

### 3. Operator Equations

Suppose we are playing a game and the rules of the game specify that we throw a die, but instead of using the value that results, we use the square of the value instead. Call the value on the die  $d$  and square of the value  $s$ . i.e.  $s = d^2$ . We can model this as follows.

$$\begin{aligned} \mathbf{D} e_d &= d e_d \\ \Rightarrow \mathbf{D}(\mathbf{D} e_d) &= d \mathbf{D} e_d = d^2 e_d \end{aligned} \tag{9}$$

Remember that  $\mathbf{D}$  is just a matrix. We can apply it twice to a vector or we can square it and apply the result of the matrix squared.

$$\Rightarrow \mathbf{D}(\mathbf{D} v) = \mathbf{D}^2(v) \tag{10}$$

Using this rule in (9) we get.

$$\mathbf{D}^2 e_d = d^2 e_d \tag{11}$$

Clearly we can extend this to model any power of the eigenvalue. We can add powers together to build polynomials.

$$(\mathbf{D}^3 + \mathbf{D}^2 + 5\mathbf{I}) e_d = (d^3 + d^2 + 5) e_d \tag{12}$$

We can even take suitably convergent infinite series such as exponentials or trigonometric functions.

$$\left(\mathbf{D} - \frac{1}{3!}\mathbf{D}^3 + \frac{1}{5!}\mathbf{D}^5 + \dots\right)e_d = \sin(\mathbf{D})e_d = \sin(d)e_d \quad (13)$$

Diagonal matrices like the  $\mathbf{D}$  operator, are easy to manipulate this way: if you multiply a diagonal matrix by itself you just get another diagonal matrix. e.g.

$$\mathbf{D}^2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 36 \end{bmatrix} \quad \sin(\mathbf{D}) = \begin{bmatrix} \sin(1) & 0 & 0 & 0 & 0 & 0 \\ 0 & \sin(2) & 0 & 0 & 0 & 0 \\ 0 & 0 & \sin(3) & 0 & 0 & 0 \\ 0 & 0 & 0 & \sin(4) & 0 & 0 \\ 0 & 0 & 0 & 0 & \sin(5) & 0 \\ 0 & 0 & 0 & 0 & 0 & \sin(6) \end{bmatrix} \quad (14)$$

However, even if the matrix is not diagonal, we can still take powers and form power series.

If we give a name to the  $\mathbf{D}^2$  operator, call it  $\mathbf{S}$  say, then the numeric equation:

$$d^2 = s \quad (15)$$

Can be replicated in the operator equation:

$$\mathbf{D}^2 e_d = \mathbf{S} e_d \quad (16)$$

This ability to manipulate operators in many of the same ways as we do numbers, enables us to build equations from operators. We will use this in the final section of this paper to build the Schrödinger equation.

#### 4. Comparing Vectors and Introducing Dirac Notation

One of the things we can do in geometry is compare one vector to another by forming their **dot product**. You will probably be familiar with the formula:

$$\vec{a} \cdot \vec{b} = |\vec{a}||\vec{b}|\cos(\theta) = \sum a_i b^i \quad (17)$$

We can use the sum of components version to generalise this to vectors of any dimension.

Notice that the components on vector  $b$  are given upper indices and the components on  $a$  are given lower indices. Basically, upper indices means they are components of a column vector and lower indices means they are components of a row vector.<sup>2</sup> So one way of writing the dot product of two 3D vectors would be:

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<sup>2</sup> You might see column vector components being referred to as **contravariant** and row vector components as **covariant**. If you want to remember which ones are upper and which ones are lower indices, just remember that “co is low”.

$$\vec{a} \cdot \vec{b} = \begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} \begin{bmatrix} b^1 \\ b^2 \\ b^3 \end{bmatrix} . \quad (18)$$

In our examples so far, upper and lower indexed components are numerically identical, just arranged vertically or horizontally when written out. We will see examples shortly where this is not the case.

The dot product is a measure of how similar two vectors are. If  $a$  and  $b$  are vectors that point in the same direction then the result is just the product of their magnitudes. If  $a$  and  $b$  are at right angles then their dot product is zero. As we are representing states of a random variable by vectors, the dot product therefore gives us a handy way of comparing two states.

Because the dot product compares two vectors it is sometimes referred to as the **overlap** between them: the bigger the overlap between their components, the more similar they are. This is a description that I will use a lot.

At this point it is worth switching to **Dirac notation**. This was introduced by Paul Dirac in his seminal work on quantum mechanics [1]. In Dirac notation, the vector  $e_i$  is written  $|i\rangle$  and instead of being called a column vector it is called a **ket**. The terms “vector” and “ket” are used interchangeably. So in Dirac notation, the eigenvalue equation for our simple die is written:

$$D|n\rangle = n|n\rangle \quad (19)$$

where  $|n\rangle$  is a column vector. The corresponding row vector is written  $\langle n|$  and is called a **bra**. So for example:

$$\text{ket } |2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \leftrightarrow \quad \text{bra } \langle 2| = [0 \ 1 \ 0 \ 0 \ 0 \ 0] \quad (20)$$

Instead of writing the overlap of two vectors as  $a \cdot b$ , we write them instead as a bra and a ket back to back:  $\langle a|b\rangle$ . This is called a **bra-ket** (this was Dirac’s little joke). Here are a couple of examples.

$$\langle 1|1\rangle = [1 \ 0 \ 0 \ 0 \ 0 \ 0] \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 1 \quad \langle 1|2\rangle = [1 \ 0 \ 0 \ 0 \ 0 \ 0] \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0 \quad (21)$$

As you can see the overlap of  $\langle 1|$  with itself,  $|1\rangle$ , is unity. It's overlap with any other basis ket is zero.

*Aside.* You might want to think about what happens when we multiply a column vector into a row vector. For a two dimensional vector space we get the following matrix.

$$|a\rangle\langle b| = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \begin{bmatrix} b^1 & b^2 \end{bmatrix} = \begin{bmatrix} a_1 b^1 & a_1 b^2 \\ a_2 b^1 & a_2 b^2 \end{bmatrix} \quad (22)$$

If you do this with the basis vectors you get the following.

$$\begin{aligned} |1\rangle\langle 1| &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\ |2\rangle\langle 2| &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \end{aligned} \quad (23)$$

We can add these two matrices together.

$$|1\rangle\langle 1| + |2\rangle\langle 2| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I \quad (24)$$

The general expression

$$\sum_i |i\rangle\langle i| = I \quad (25)$$

where  $i$  is over the dimension of the vector space, is used frequently in QM.

If we multiply  $|i\rangle\langle i|$  by the corresponding eigenvalue, and sum over all values of  $i$ , we get the measurement operator. For example, for the die measurement operator:

$$D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 \end{bmatrix} = 1|1\rangle\langle 1| + 2|2\rangle\langle 2| + \dots + 6|6\rangle\langle 6| \quad (26)$$

## 5. Kets and Probabilities

Let's look at the state  $|3\rangle$ . This represents the state where the die has come to rest with the value 3 face up. This is a completely known state, so the probability of observing a 3 if we look at it again is 1. The probability of all other values is zero. But these are precisely the components of  $\langle 3| = (0,0,1,0,0,0)$ . (We're showing the row vector for convenience.) This suggests that we can relate the components of a ket to the probabilities of the possible states.



Most of the time, we will want to calculate the probability of a particular state given its current state. i.e. The *conditional probability* that we described in section 1. To compare one state to another we take their overlap. The maximum overlap happens when the two vectors are identical, while an overlap of 0 means they have nothing in common at all.

If the die has come to rest in a state  $|i\rangle$ , we can ask if it is in the state  $|3\rangle$  by forming its overlap with  $|3\rangle$ .  $\langle 3|i\rangle = 1$  if the die is in state  $|3\rangle$ , and it is zero if the die is in any other state. These are exactly the conditional probabilities we would expect: if the die has landed and is in the state  $|3\rangle$ , then the probability of finding it in state  $|3\rangle$  is clearly 1 and the probability of finding it in any other state is zero.

So far, the only states of our die that we have identified are the states corresponding to the basis kets  $|i\rangle$ , where the die has come to rest and the number  $i$  is showing face up. How would we represent the state where the die has just been thrown, it is tumbling unpredictably through the air, and the final outcome is unknown?

Let us define the following state.

$$|u\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad (27)$$

The “u” stands for “unknown”. This is quite different from all the states we have seen so far. It isn’t an eigenstate of the  $D$  operator. It has equal amounts of “oneness” “twoness” and so on. Such a general combination of the basis vectors is called a **state vector** or a **state ket**. These can be basis vectors or any linear combination of basis vectors.

First look at the fraction that multiplies the ket. This is chosen so that if we calculate the overlap of  $|u\rangle$  with itself we get  $\langle u|u\rangle = 1$ . This is consistent with our interpretation of the overlap as a conditional probability. The probability of the die being in the state  $|u\rangle$ , given that it is already in the state  $|u\rangle$ , is:  $P(u | u) = \langle u|u\rangle = 1$ .

When  $\langle u|u\rangle = 1$ , we say it that  $|u\rangle$  is **normalised**. This condition guarantees the correct conditional probability when we take the overlap of a vector with itself. We can always put a constant in front a state vector so that it is normalised, i.e. its overlap with itself is 1.

Suppose the die is in the state  $|u\rangle$ . Can we get the probability of it ending up in the state  $|3\rangle$  say? If we first take the overlap between the two states, we get.

$$\langle 3|u\rangle = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{6}} \quad (28)$$

To get the correct probability we have to square this.

$$\langle 3|u\rangle^2 = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}^2 = \frac{1}{6} \quad (29)$$

The reason we have to square the overlap is simple. Consider a normalised state

$$\langle x| = (a, b, c, \dots).$$

As it is normalised,  $\langle x|x\rangle = 1$ . i.e.

$$\langle x|x\rangle = \begin{bmatrix} a & b & c & \dots \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ \vdots \end{bmatrix} = a^2 + b^2 + c^2 + \dots = 1 \quad (30)$$

So it is the sum of the *squares* of the components that equals 1. Clearly the probability distribution is also formed from these squares. i.e.  $P(a) = a^2$ .

Now suppose we take the overlap of  $|x\rangle$  with one of the basis vectors.

$$\langle 1|x\rangle = \begin{bmatrix} 1 & 0 & 0 & \dots \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ \vdots \end{bmatrix} = a \quad (31)$$

i.e. The overlap gives us the result,  $a$ , which we know is not the probability of  $a$ . So we take its square instead. (The reason we didn't have to square things in the previous examples is simply because  $1^2 = 1$  and  $0^2 = 0$ , so squaring would make no difference.)

Clearly, we can compute probabilities of any of the six die values in a similar way. In this case, no matter what eigenvector of  $D$  we use, we will always get the value  $1/6$ .

This generalises quite easily. If the die is in state  $|b\rangle$  (normalised to 1) and we want to know the probability that we will measure state  $|a\rangle$  (also normalised to 1), then we just compute  $\langle a|b\rangle^2$ . In symbols:

$$P(a | b) = \langle a | b \rangle^2.$$

As another example, suppose the die has almost come to rest and the outcome is not quite certain but it's going to be one of: 1, 3 or 5, with the first two being even more likely. The probable outcomes might be reflected in a state vector like the following:

$$|s\rangle = \frac{1}{3} \begin{bmatrix} 2 \\ 0 \\ 2 \\ 0 \\ 1 \\ 0 \end{bmatrix}. \quad (32)$$

The probability of 3 landing face up is now.

$$\langle 3|s\rangle^2 = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \frac{1}{3} \begin{bmatrix} 2 \\ 0 \\ 2 \\ 0 \\ 1 \\ 0 \end{bmatrix}^2 = \frac{4}{9} \quad (33)$$

This brings us to the second postulate that is found near the start of most QM textbooks.

***The state of a system in quantum mechanics is represented by a state vector. The probability of any given measurement is given by the square of the overlap between the state vector and the corresponding eigenvector.***

Again, if you haven't seen this before, it can seem like a deeply mysterious statement. But as you can see, any random variable whose possible outcomes are encoded as a vector space, will demonstrate similar properties.

## 6. Probability Amplitudes

As seen above, the state vector can be viewed as a kind of square root of a probability distribution. It is sometimes referred to as a **probability amplitude**, although the term can also be used for an individual component of the state vector. This is yet another name that refers to exactly the same object as a "ket", which is the same as a "state vector" (which is the same as a "wavefunction", but we haven't used that term yet). They're all the same thing. When one term is used rather than another it is just to emphasise a particular aspect of the same object. So if someone refers to a "state vector" then they probably intend to concentrate on its properties as an element of a vector space. If

the same object is referred to as a “probability amplitude” then it is because they want to emphasise that it is the square root of a probability distribution.

Sometimes we want to find the probability amplitude for a state that is some composite of the eigenstates. The  $|u\rangle$  state is an example of this. Let us return to the example where someone throws the die, allows it to land and then observes its value, but they only tell us that the value is an even number. To construct a representation of this state we simply take all the possible even states, add them together, and normalise the result.

$$|2\rangle + |4\rangle + |6\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \rightarrow |e\rangle \equiv \frac{1}{\sqrt{3}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

Our rule for calculating probabilities remains the same: take the overlap with the state whose probability we want, and square the result. For example, if we want the probability of the value being 6, given that the state is known to be even:

$$\langle 6|e\rangle^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \frac{1}{\sqrt{3}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}^2 = \frac{1}{3}$$

which is exactly what we would expect.

What about the probability of throwing an even value in the first place? Again, we apply our rule of taking the overlap of the even state with the unknown state:

$$\langle e|u\rangle^2 = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix} \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}^2 = \left[ \frac{3}{\sqrt{3}\sqrt{6}} \right]^2 = \frac{1}{2}$$

The normal rule for adding probabilities is to take the probabilities of the individual, mutually exclusive, independent events, and add them together. There are three events that give an even number: namely throwing the values 2, 4 or 6, each with a probability of 1/6. Adding these probabilities together gives  $3 \times 1/6 = 1/2$ . This is the same as we obtained by creating the even state,  $|e\rangle$ , by adding the amplitudes, and then applying our overlap squared rule. As we will see later, this is not always the case in QM, and this is one of the things that makes the subject so interesting.

The even state,  $|e\rangle$ , is an example of the *superposition rule*: if a condition can be reached in more than one way, then add together all the probability amplitudes that correspond to that condition to get the correct state.

This rule is used all the time in QM. For example, in the double slit experiment, where a photon can arrive at a location via two distinct routes, we add the amplitudes for those two routes to determine the probability that it will arrive at the final destination.

## 7. The Meaning of Superpositions and the Collapse of the Wavefunction

The exact meaning of states that are superpositions of eigenstates is not always well defined. Suppose we are told that the die is in the  $|u\rangle$  state. We previously interpreted this state as the die tumbling through the air. In this case it genuinely is not in one of the eigenstates of the die measurement operator,  $\mathbf{D}$ .

However, suppose the die lands and is immediately covered with a cloth so that we cannot see its value. The die now has a definite value, it is in one of the  $\mathbf{D}$  operator eigenstates, we just don't know which one. To calculate probabilities, we have to treat the die as if it is still in the  $|u\rangle$  state because we have no idea which state it is really in. So the  $|u\rangle$  state can represent two distinct physical situations. There is the case where it is genuinely not in an eigenstate of the  $\mathbf{D}$  operator, and there is the case where it *is* in an eigenstate of the  $\mathbf{D}$  operator but our lack of knowledge means we have to treat it as if it is in the  $|u\rangle$  state.

The formalism presented so far cannot distinguish between these two cases, yet the distinction is vital. A die tumbling through the air evolves quite differently over time to a die that is stationary and covered by a cloth. This is true in general. A system in a superposition of states will usually evolve in time quite differently from a system in a particular eigenstate.

In most situations in QM we have to deal with a system which is in a genuine superposition of states. Indeed, we will see shortly that most quantum systems are *always* in a superposition of states. ***This is arguably the single most unique and important aspect of QM, that systems are normally in a state where they have multiple positions, multiple momenta, multiple energies, multiple just about everything.***

In the die example, the die is initially in a superposition of eigenstates,  $|u\rangle$ . While in the state,  $|u\rangle$ , the die has no definite value. Eventually it comes to rest in one of the eigenstates  $|i\rangle$ . We then observe which eigenstate it is in and measure a definite value. This change from a superposition to an eigenstate is often referred to as the “collapse of the wavefunction”.

In the case of the die, the collapse of the wavefunction is trivial, it is simply a reflection of the die coming to rest. We have only defined one type of measurement, namely the value on the die, and one type of eigenstate. When we come to systems with more than one measurement operator, and different sets of eigenstates, this becomes much more interesting.

In QM, the act of measurement itself forces a system into an eigenstate of the corresponding measurement operator. If we are determined to measure a position then the system will oblige by moving from a state which is a superposition of position states, into a state with a definite position. This is often expressed as a postulate of QM.

***A measurement of a system causes the state of the system to collapse from a superposition of states into an eigenstate of the corresponding measurement operator.***

On the basis of our only example so far, this does not seem like a particularly profound statement. However, the effect in QM can be very strange.

For example, you will find in your QM course that a moving electron is in a wave like eigenstate of momentum (we will briefly explore this later). A stationary electron, on the other hand, adopts a single large “spike” corresponding to its single, fixed, position. So when a moving electron is brought to rest so that its position can be measured, it moves from the wave like momentum eigenstate, to the spike-like position eigenstate. In this case, the “collapse of the wavefunction” is really just a switch from an eigenstate of momentum to an eigenstate of position. This has been summarised by some as “electrons propagate as waves but interact as particles.”

A good example of the weirdness of wave function collapse is illustrated by the Einstein, Podolsky, Rosen problem.[7] Two particles with zero total angular momentum go off in opposite directions. A measurement of the spin of one collapses the wave function for the two particle system. This then instantaneously affects the spin measurement of the other particle, no matter how far apart they are. Experiment confirms that this really does happen, and due to a theorem by John Bell, it can be shown that no “local hidden variable” can account for this.[8]

There doesn't appear to be any obvious classical analogy of this kind of behaviour. I think it's safe to say that the collapse of the wavefunction is an aspect of QM that is not yet fully understood.

## 8. Tossing a Coin

We now consider the toss of a coin that can land either heads up or tails up. On the face of it this looks like a much simpler situation than the six sided die. However, it will allow us to examine several additional aspects of this type of probability model.

As there are two possible measurements, we choose to represent them by a two dimensional vector space. Heads and tails are represented as follows.

$$|h\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |t\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (34)$$

Our measurement operator has the following form. ('H' stands for Heads or tails.)

$$\mathbf{H} = \begin{bmatrix} h & 0 \\ 0 & t \end{bmatrix} \quad (35)$$

Here,  $h$  and  $t$  can take on any two distinct values. I will choose the values +1 and -1 respectively. As before, our measurement operator satisfies the eigenvalue equations.

$$\begin{aligned} \mathbf{H} |h\rangle &= h |h\rangle \\ \mathbf{H} |t\rangle &= t |t\rangle \end{aligned} \quad (36)$$

Suppose the coin is set spinning clockwise on its edge on a table. It is neither in an  $|h\rangle$  state or a  $|t\rangle$  state but has equal probability of ending up in either. We will label this state as  $|c\rangle$ .

$$|c\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (37)$$

$\langle c|c\rangle = 1$  as required by a normalised state vector, and  $P(h|c) = \langle h|c\rangle^2 = P(t|c) = \langle t|c\rangle^2 = 1/2$ , exactly as expected.

Now consider the following state vector.

$$|a\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (38)$$

This has all the same important overlaps as  $|c\rangle$ :  $\langle a|a\rangle = 1$ ,  $\langle h|a\rangle^2 = \langle t|a\rangle^2 = 1/2$ . Yet  $|c\rangle$  and  $|a\rangle$  are clearly very different vectors. In fact, they are orthogonal.

$$\langle a|c\rangle = \frac{1}{\sqrt{2}} [1 \quad -1] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \quad (39)$$

They also form a complete set: any vector can be expressed as some combination of  $|c\rangle$  and  $|a\rangle$ . To see this we show that  $|h\rangle$  and  $|t\rangle$  can be formed from  $|c\rangle$  and  $|a\rangle$ :

$$\begin{aligned} |h\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} |c\rangle + \frac{1}{\sqrt{2}} |a\rangle, \\ |t\rangle &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} |c\rangle - \frac{1}{\sqrt{2}} |a\rangle. \end{aligned} \quad (40)$$

As any vector can be formed from  $|h\rangle$  and  $|t\rangle$  it follows that any vector can be formed from  $|c\rangle$  and  $|a\rangle$ :

$$\begin{bmatrix} a \\ b \end{bmatrix} = a|h\rangle + b|t\rangle = a \left( \frac{1}{\sqrt{2}} |c\rangle + \frac{1}{\sqrt{2}} |a\rangle \right) + b \left( \frac{1}{\sqrt{2}} |c\rangle - \frac{1}{\sqrt{2}} |a\rangle \right). \quad (41)$$

$|c\rangle$  and  $|a\rangle$  are also eigenvectors of the following operator:

$$\mathbf{S} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (42)$$

$$\mathbf{S}|c\rangle = +1|c\rangle \quad \mathbf{S}|a\rangle = -1|a\rangle$$

So  $|c\rangle$  and  $|a\rangle$  are orthogonal, they form a complete set and they are the eigenvectors of the  $\mathbf{S}$  operator. The  $\mathbf{S}$  operator looks like it represents a measurement, but a measurement of what? I choose to have it represent the coin Spinning on its edge with two possible states: spinning Clockwise (the  $|c\rangle$  state) or spinning Anti-clockwise (the  $|a\rangle$  state).

You might quite legitimately ask, how can I simply choose the operator and eigenvectors to mean whatever I want them to mean? Actually we have been making these sort of choices all along. The die operator,  $D$ , didn't have to have all the numbers 1...6 in order, they could have been jumbled up. They didn't even have to be the numbers 1...6, we could have chosen any distinct set of numbers and kept a mapping between those and the values on the die. All that mattered was that the dimension of the vector space matched the number of possible measurements. As long as we applied this consistently everything would still work.

One of the differences between these simple examples and QM, is that in QM the measurement operators have meanings that are dictated by physics, not by our arbitrary choices.

We now have two measurement operators,  $H$  and  $S$ , that can act on the same set of state vectors. These two operators have different sets of eigenvectors. This means that if the coin is in a definite  $H$  state (showing a definite side, i.e.  $|h\rangle$  or  $|t\rangle$ ), then it cannot simultaneously be in a definite  $S$  state (spinning one way or the other i.e.  $|c\rangle$  or  $|a\rangle$ ). The converse is equally true: if the coin is spinning then it is not showing a definite side. This is the origin of the famous **Heisenberg uncertainty principle**. Wherever there are two measurement operators, acting on the same space of state vectors, but with mutually exclusive sets of eigenvectors, the uncertainty principle will come into play.

Notice that the  $H$  and  $S$  operators do not commute.

$$\begin{aligned} HS &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \\ SH &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = -HS \end{aligned} \tag{43}$$

It's easy to show that operators that share the same eigenvectors commute. Suppose  $A$  is an operator with eigenvectors  $|e_k\rangle$  and eigenvalues  $a_k$ . Now let  $B$  be a different operator, sharing the same eigenvectors but with eigenvalues  $b_k$ . Then

$$\begin{aligned} A|e_k\rangle &= a_k|e_k\rangle \\ \Rightarrow BA|e_k\rangle &= B a_k|e_k\rangle = a_k B|e_k\rangle = a_k b_k|e_k\rangle \end{aligned} \tag{44}$$

but

$$\begin{aligned} B|e_k\rangle &= b_k|e_k\rangle \\ \Rightarrow AB|e_k\rangle &= A b_k|e_k\rangle = b_k A|e_k\rangle = b_k a_k|e_k\rangle \end{aligned} \tag{45}$$

As  $b_k$  and  $a_k$  are just numbers that commute,  $AB$  and  $BA$  always have the same effect.

If the two operators  $A$  and  $B$  do not share any eigenvectors, then it is equally easy to show that they do not generally commute. Suppose.

$$A|e_k\rangle = a_k|e_k\rangle \tag{46}$$



We are now assuming that  $|e_k\rangle$  are not eigenvectors of  $\mathbf{B}$ . So when  $\mathbf{B}$  acts on one of them it does not return the same vector back. However the  $|e_k\rangle$ 's form a complete set, so the result of  $\mathbf{B}$  acting on one of them will return a vector that can be built from some linear combination of  $|e_k\rangle$ 's.

$$\begin{aligned} \mathbf{B}|e_k\rangle &= \sum c_i |e_i\rangle \\ \Rightarrow \mathbf{A}\mathbf{B}|e_k\rangle &= \mathbf{A} \sum c_i |e_i\rangle = \sum c_i \mathbf{A}|e_i\rangle = \sum c_i a_i |e_i\rangle \end{aligned} \quad (47)$$

but

$$\begin{aligned} \mathbf{A}|e_k\rangle &= a_k |e_k\rangle \\ \Rightarrow \mathbf{B}\mathbf{A}|e_k\rangle &= \mathbf{B} a_k |e_k\rangle = a_k \mathbf{B}|e_k\rangle = a_k \sum c_i |e_i\rangle \neq \sum c_i a_i |e_i\rangle \end{aligned} \quad (48)$$

The **commutator** of two operators is defined as:

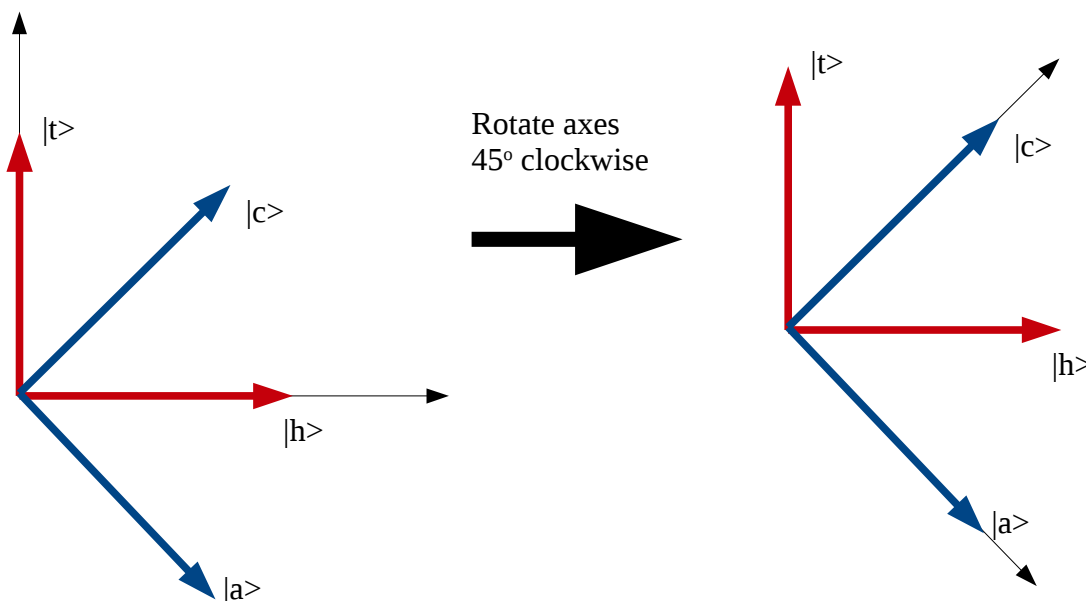
$$[\mathbf{H}, \mathbf{S}] \equiv \mathbf{H}\mathbf{S} - \mathbf{S}\mathbf{H} \quad (49)$$

The fact that they do not commute can therefore be expressed as:

$$[\mathbf{H}, \mathbf{S}] \neq 0 \quad (50)$$

You will find that the relationship between two operators is often expressed in terms of their commutator.

Notice that only  $\mathbf{H}$  is diagonal, with “simple” eigenvectors. There is nothing special about the  $\mathbf{H}$  operator. We could choose to make the  $\mathbf{S}$  operator diagonal instead. Imagine  $|h\rangle$  and  $|t\rangle$  as normal 2D vectors lying along the x and y axes. We can rotate the x and y axes 45° clockwise so that they lie along the  $|a\rangle$  and  $|c\rangle$  vectors instead. The  $\mathbf{S}$  operator will then be diagonal with eigenvectors corresponding to the basis vectors, and  $\mathbf{H}$  will have the more complicated form.

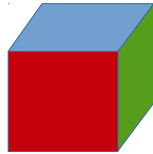


## 9. The Pauli Matrices and Complex Numbers

The coin provided an example of two measurement operators acting on the same set of two dimensional vectors. We're now going to look at an example of three measurement operators acting on a two dimensional vector space. Now it gets really interesting.

In this example, take a six sided die, paint three adjacent sides red, blue and green, and their opposite sides black. When we throw the die and it lands and comes to rest, it will therefore be in one of the following states:

1. Red facing up.
2. Red facing down.
3. Blue facing up.
4. Blue facing down.
5. Green facing up.
6. Green facing down.



We will model this as three separate measurements: red up or down, blue up or down, and green up or down. i.e. We have three mutually exclusive measurements, each of which has two possible states.

We've already seen how to model a two state observable in the coin tossing example and can follow a similar course here. We take a two dimensional vector space and arbitrarily assign the eigenvalue +1 to the state where red is facing up and -1 to the state where red is facing down. We will call its measurement operator  $\mathbf{R}$  and it's eigenvectors  $|r+\rangle$  and  $|r-\rangle$  corresponding to red face up and red face down.

$$\begin{aligned} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} &= +1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} &\rightarrow \mathbf{R}|r+\rangle = +1|r+\rangle \\ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} &= -1 \begin{bmatrix} 0 \\ 1 \end{bmatrix} &\rightarrow \mathbf{R}|r-\rangle = -1|r-\rangle \end{aligned} \tag{51}$$

Just as with the tumbling coin example, we can easily model a second, mutually exclusive measurement, blue, using the same basis vectors.

$$\begin{aligned} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} &= +1 \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} &\rightarrow \mathbf{B}|b+\rangle = +1|b+\rangle \\ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} &= -1 \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} &\rightarrow \mathbf{B}|b-\rangle = -1|b-\rangle \end{aligned} \tag{52}$$

Note that, by symmetry, the magnitude of the “red up” and “red down” components in the blue eigenstates must be equal.

However, if we want to include the third measurement operator, the green up or down operator, then we have a problem. Again, by symmetry the magnitude of the green eigenstates’ “red up” and “red down” components must be equal. But this would make them just a multiple of the blue eigenstates

when they should really be equal magnitude sums of them as well. There appears to be no way to include a third measurement operator – we’ve run out of numbers. The solution is to extend the allowed numbers in our vectors from the real numbers to the complex numbers (the following choice is not unique, but it’ll do the job).

$$|g+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \quad |g-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} \quad (53)$$

Note that, to get  $\langle g+|g+\rangle = 1$  and  $\langle g+|g-\rangle = 0$ , we have to modify our rule for creating kets from bras. It’s not enough to turn the column vector into a row vector, we must also take the complex conjugates of the components as well.

$$\begin{aligned} \langle g+|g+\rangle &= \frac{1}{\sqrt{2}} [1 \quad i]^* \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{\sqrt{2}} [1 \quad -i] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = 1 \\ \langle g+|g-\rangle &= \frac{1}{\sqrt{2}} [1 \quad i]^* \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{\sqrt{2}} [1 \quad -i] \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} = 0 \end{aligned} \quad (54)$$

In general, the overlap between two vectors can now be a complex number. To convert this to the probability of a particular outcome we must first take the absolute magnitude of the overlap before squaring it. For example, if the die is in an arbitrary state  $|a\rangle$  and we want to calculate the probability that we measure  $|g+\rangle$  then we must do the following.

$$|\langle g+|a\rangle|^2 = \left| \frac{1}{\sqrt{2}} [1 \quad i]^* \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \right|^2 = \frac{1}{2} |a_1 - ia_2|^2 \quad (55)$$

It can easily be shown that this rule works in general.

The presence of complex components means that we must now allow complex coefficients when adding together vectors. For example:

$$|g+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1+i}{2} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{1-i}{2} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1+i}{2} |b+\rangle + \frac{1-i}{2} |b-\rangle \quad (56)$$

The green measurement operator now takes the form:

$$\mathbf{G} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad (57)$$

It’s action on the green eigenstates is as expected:

$$\begin{aligned} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} &= +1 \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} &\rightarrow G|g+\rangle = +1|g+\rangle \\ \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} &= -1 \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} &\rightarrow G|g-\rangle = -1|g-\rangle . \end{aligned} \tag{58}$$

We can relabel our three measurement operators as follows (the reason for relabelling them is so that we can refer to them by an index).

$$\sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{59}$$

These are the famous **Pauli matrices**. They are ubiquitous in any discussion of spin-1/2 particles. They have numerous interesting properties that you will explore in your QM course.

## 10. Continuous Distributions

Let's go back to our normal die. Instead of the value that lands face up on our die, suppose we are interested in the horizontal position where the die lands on the table. We can suppose that the table is marked with equally spaced 5 cm strips and that the die always lands wholly within one of those strips. If the table is one metre long then there will be 20 possible positions where the die can land, so we will need a 20 dimensional vector space to model it.

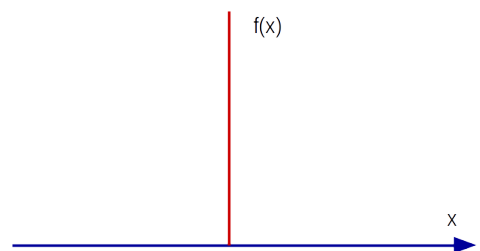
$$\begin{bmatrix} 5 & 0 & \dots & 0 \\ 0 & 10 & & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \dots & 100 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix} = 10 \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix} \tag{60}$$

If we refine our distance measurement further, to a resolution of 1cm, then we will need a 100 x 100 measurement matrix and a 100 component vector. In the limit, the state goes from a discrete vector to a continuous function,  $f(x)$ . The position operator  $X$  is then defined as follows.

$$X f(x) = x f(x) \tag{61}$$

This should be read as the position operator  $X$ , acting on the state  $f(x)$ , returns the position  $x$  times the state  $f(x)$ . It has exactly the same form as the discrete eigenvalue equation. Unlike the examples we have been using so far, this really is an operator equation from QM.

Our previous die eigenstates consisted of vectors that had five zeroes and one value where all the probability was concentrated. Similarly, the eigenfunctions of equation (61),  $f(x)$ , are zero everywhere except at a single infinitely thin, infinitely high, spike. (These are called **Dirac delta functions**.)



We obtained these from a limiting procedure. In reality, physical objects do not occupy a single position<sup>3</sup>. Our die is not a mathematical point. It occupies a small range of positions with a width determined by its orientation. So its real physical state must be represented by a sum of position eigenstates. We will see the need to use sums of eigenstates repeatedly in what follows.

Just as with discrete state vectors, we form the overlap by summing all the components. In the limit that state vectors become functions, the components are just the values of the functions themselves. So if  $|a\rangle$  and  $|b\rangle$  are now functions (we use Dirac notation to label functions as well as vectors) then the overlap is now given by:

$$\langle a|b\rangle = \int a(x)b(x)dx \quad . \quad (62)$$

Just as with state vectors, these functions must be normalised.

$$\langle a|a\rangle = \int a(x)a(x)dx = 1 \quad . \quad (63)$$

With discrete vectors, the square of the components gave a probability distribution. With continuous functions, the square of the function gives a **probability density function**.

Differential operators are linear operators. For example, if  $f(x)$  and  $g(x)$  are two functions of  $x$ , then:

$$\frac{\partial}{\partial x}(af + bg) = a\frac{\partial}{\partial x}f + b\frac{\partial}{\partial x}g \quad . \quad (64)$$

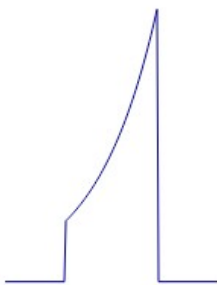
Can we interpret differential operators as measurement operators? Up until now we have known exactly what our measurement operators represented. Here we have a candidate for a measurement operator, but we have no idea what the derivative of the square root of a probability distribution could possibly represent. To find out we have to just go with it and see what turns up.

If we write down the eigenvalue equation for the derivative operator:

$$\frac{\partial}{\partial x}f(x) = k_f f(x) \quad (65)$$

where  $k_f$  is the eigenvalue specific to the function  $f$ . The solution is:

$$f(x) = e^{k_f x} \quad . \quad (66)$$



If  $k$  is real, as we expect measurement eigenvalues to be, then this has several problems as a probability amplitude. It cannot be normalised over  $(-\infty, \infty)$  and has to be normalised over a fixed interval instead. But if we only look at the function over a fixed interval, we end up with something like the diagram to the left. There are continuity problems at the edges of this interval where the function must suddenly jump to zero.

<sup>3</sup> Quantum field theory does represent particles as mathematical points, but this leads to its own problems.

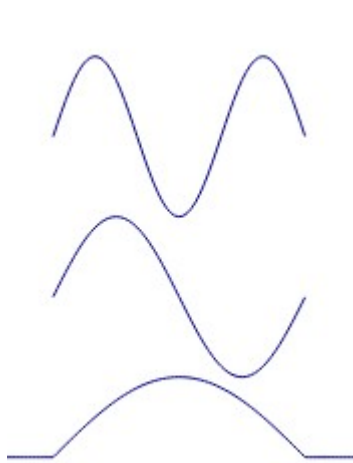
The principal problem however is the inability to construct an orthogonal set of eigenvectors. If  $m$  and  $n$  are two real eigenvalues then, regardless of the range of integration.

$$\langle m|n\rangle = \int e^{mx} e^{nx} dx \neq 0 \quad (67)$$

However, if we allow the exponent to be imaginary then things are very different.

$$f(x) = e^{ikx} = \cos(kx) + i \sin(kx) \quad (68)$$

This is still not normalisable over  $(-\infty, \infty)$ . However, with suitable boundary conditions, and taking appropriate linear combinations of solutions (e.g.  $ie^{-ikx} - ie^{ikx} = 2 \sin(kx)$ ), it can at least be arranged to be zero at the ends of a finite interval, thus providing continuity with the value zero outside the chosen interval. In many cases this requirement will only work for complete half cycles of the  $\sin$  or  $\cos$  functions, leading to **quantisation** of the allowed values of the space derivative operator.



It's worth noting that we had to take a sum of two eigenstates to get a workable solution. A single eigenstate by itself would not satisfy reasonable boundary conditions.

Another advantage of the  $ie^{ikx}$  solutions is that they have constant magnitude of one:  $|ie^{ikx}| = 1$ . If we want to construct an equal probability density function then this property is essential. Clearly this cannot be with real trigonometric functions.

In order to get a real eigenvalue, which we require in order to treat it as an observable measurement, we have to modify the differential operator.

$$-i \frac{\partial}{\partial x} e^{ikx} = -i(ik) e^{ikx} = k e^{ikx} \quad (69)$$

Just as when complex numbers became part of our discrete vectors, our definition of the overlap must now change:

$$\langle a|b\rangle = \int a^*(x) b(x) dx \quad (70)$$

Notice that, once again, complex numbers have made their way into the theory for quite prosaic reasons: *if* the differential operator represents an observable quantity then we need complex numbers to prevent the probability amplitudes associated with it from being exponential. This in turn implies that there is a “wavy” aspect to any such probability amplitude. In the die example this is clearly unexpected and quite counter-intuitive: there doesn't seem to be anything even remotely “wavy” about a die. It is this wavy aspect that leads to the term **wavefunction** to describe states (to add to state vector, state ket, and probability amplitude). We will see shortly that the position derivative eigenstates have a surprising physical interpretation.

Note that we can still have arbitrary probability amplitudes of position. It is only the eigenstates of the position derivative that are now being constrained. Provided these form a complete set (which they do), then just as with the discrete eigenvectors for the die value, we can still built any probability amplitude we please from them.

If the probability amplitudes vary with time as well as space, then the derivative with respect to time is also a linear operator. Just as we did for the position derivative operator, we can define an eigenvalue equation for the time derivative operator. For exactly the same reason, the eigenfunctions of the time derivative must also be complex and we get the time derivative equation.

$$i \frac{\partial}{\partial t} e^{-i\omega t} = i(-i\omega) e^{-i\omega t} = \omega e^{-i\omega t} \quad .^4 \tag{71}$$

We can combine the time and space solutions to get the standard wave equation.

$$f(x, t) = e^{i(kx - \omega t)} \tag{72}$$

The time derivative eigenvalues also turn out to have a surprising physical interpretation.

## 11. Quantum Mechanics

To summarise so far. If we take a random variable, with a discrete set of possible values, and map this set to the basis of a finite dimensional vector space, we quickly discover that the resultant state vectors can be treated like probability amplitudes. The overlap between two vectors allows us to compare states, and the square of the overlap between a basis vector and an arbitrary state gives us the probability of measuring the value corresponding to the basis vector.

The possible outcomes of a measurement are given by the eigenvalues of its measurement operator. The value of a measurement is only certain when the state is one of the measurement operator's eigenvectors.

If two or more measurement operators share the same set of state vectors, but have different sets of eigenvectors, then the two measurements cannot be known simultaneously.

If we have three measurement operators each with only two states of equal probability then we must introduce complex numbers in order to give the third measurement operator its own eigenvectors.

We can treat continuous variables as the limit of this process. The partial derivatives of continuous amplitudes are candidates for measurement operators. However the eigenvalue equations of derivative operators lead to exponential solutions unless we once again introduce complex numbers.

We can establish all of the above without a single experiment. To progress from an abstract mathematical theory to QM we must now include some physics. We will start with the Einstein-Planck hypothesis, that the energy of a photon is given by:

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4 The “-” sign is due to the convention that we treat right moving waves as moving along the positive  $x$  axis. It's a convention that also comes in handy when we do relativistic QM and we want time and space to have opposite signatures.

$$E = h\nu = \hbar\omega \quad . \quad (73)$$

The amplitude of a wave of frequency  $\omega$  has the form:  $y = \sin(-\omega t) = \text{Im}(e^{-i\omega t})$ , which we immediately recognise as an eigenstate of the time derivative operator. To convert the time derivative operator into an energy operator, all we need is the addition of Planck's constant.

$$i\hbar \frac{\partial}{\partial t} e^{-i\omega t} = i\hbar \frac{\partial}{\partial t} e^{-iEt/\hbar} = E e^{-iEt/\hbar} \quad (74)$$

Note that, to be an eigenstate of a derivative operator, the function must be complex if we are to avoid exponential solutions.

This is one of the fundamental postulates of QM: that the energy operator is given by:

$$\mathbf{E} = i\hbar \frac{\partial}{\partial t} \quad . \quad (75)$$

Louis de Broglie took the Einstein-Planck hypothesis a step further. He wondered if the wavefunction  $e^{-iEt/\hbar}$ , in addition to applying to a photon, could also apply to a massive particle at rest.[9] It is then a simple matter to perform a Lorenz boost. The  $t$  coordinate splits into mixed time and space  $x$  coordinates, while the energy  $E$  splits into mixed energy and momentum  $p$  coefficients. This results in the wave function:

$$e^{i(px - Et)/\hbar} \quad . \quad (76)$$

Where the wavelength is given by:

$$\frac{px}{\hbar} = \frac{2\pi x}{\lambda} \Rightarrow \lambda = h/p \quad . \quad (77)$$

Once again, we see that the space part of this is just an eigenstate of the space derivative operator. As we did with time and energy, we can now define a momentum operator.

$$\mathbf{P} = -i\hbar \frac{\partial}{\partial x} \quad (78)$$

One way of looking at all of this is that we have made a number of speculative leaps whose only justification is based on whether they work or not (they do). This includes the Einstein-Planck hypothesis, the de Broglie hypothesis, and the jump from a real wave to complex eigenstates of a position probability amplitude.

Another way of looking at it is as follows.

1. The position of a particle is as valid a random variable as any other. (Remember: modelling something as a "random variable" in no way prejudices our assumptions.)
2. As demonstrated above, this inevitably means it has a position probability amplitude.



3. We define the eigenvalues of the complex time derivative operator (up to Planck's constant) to be something that we call "energy".
4. We define the eigenvalues of the complex space derivative operator (up to Planck's constant) to be something that we call "momentum".
5. We can show (as part of a QM course) that taking averages of these energy and momentum values correspond to the classical definitions of energy and momentum.

In other words, attempting to reconcile our classical notions of mechanics with QM via a series of speculations is really looking at things the wrong way round. It is QM which is the more logical model of mechanics. Classical mechanics arises from QM only as a large scale approximation.

It's worth observing that the link between the derivative operators and energy and momentum is not quite as surprising as it may at first seem. Suppose we have an infinitely differentiable function of  $x$ ,  $f(x)$ . To find the value of the function at  $f(x+\epsilon)$ , we can Taylor expand it.

$$\begin{aligned}
 f(x+\epsilon) &= f(x) + \frac{df}{dx}\epsilon + \frac{1}{2!}\frac{d^2f}{dx^2}\epsilon^2 + \dots \\
 &= \left(1 + \frac{d}{dx}\epsilon + \frac{1}{2!}\frac{d^2}{dx^2}\epsilon^2 + \dots\right) f \\
 &= \left(e^{i(-i\epsilon\frac{d}{dx})}\right) f
 \end{aligned} \tag{79}$$

i.e. We can achieve a translation in the  $x$  direction by exponentiating the  $x$  derivative operator. The  $x$  derivative operator is the **generator** of translations. We know from **Noether's theorem**, which tells us that every symmetry implies a conservation law, that translation invariance implies conservation of momentum. So there is a link between translations and momentum even in classical physics.

Similarly, the time derivative operator is the generator of (backwards) time translations and the conserved property associated with time translation invariance is energy.

We have not yet fully established the correspondence between the space derivative operator and momentum, or between the time derivative operator and energy. However, if we simply take these as further postulates of QM, we can combine them with some simple classical ideas. In particular, we can take the equation of energy conservation.

$$E = \frac{p^2}{2m} + V \tag{80}$$

where  $E$  is the total energy of a particle,  $V$  is its potential energy due to a conservative force and  $p$  is its momentum. As we indicated before, the same relationship exists between operators as between their measured values. So if we have a probability amplitude  $\Psi(x,t)$  and we act upon it with our energy and momentum operators, we get:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V\Psi(x,t) \tag{81}$$

which is the famous **time dependent Schrödinger equation**.

And now, hopefully, your QM course will make a great deal more sense.

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