

# Physics at Random

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# Chapter 1

## Linearity

Given a function  $f(x)$  and some constant  $c$ , we can ask if it matters whether we multiply the input  $x$  by  $c$  and then apply the function to the result, or we apply the function to  $x$  and multiply the result by  $c$ . That is, does this equation hold?

$$f(cx) = cf(x)$$

Or to put it another way, if we "scale up" the input, does the output scale up in proportion?

Also for two variables  $x$  and  $y$ :

$$f(x + y) = f(x) + f(y)$$

That is, it may be that it doesn't matter whether we sum the inputs and then apply the function to the sum, or apply the function to each input and then sum the results.

If both these equations hold, we say  $f$  is linear.

Actually if you take the addition rule and set  $y = x$ :

$$f(x + x) = f(x) + f(x)$$

or:

$$f(2x) = 2f(x)$$

Which is surely a huge clue about the scaling rule! Though neither is a complete statement of linearity without the other.

Sometimes these are combined into a single, albeit more confusing, requirement:

$$\mathbf{f}(ax + by) = a\mathbf{f}(x) + b\mathbf{f}(y)$$

We can generalise this concept beyond functions that act on numbers. Think of  $\mathbf{f}$  as an operator. The objects it operates on can be of any type for which we can define addition and scaling (multiplication by a constant), as that's all we need to check the linearity requirement.

We can define these capabilities for vectors, matrices and indeed all tensors, so operators acting on all those things can be linear. Now, it's easy to see how this might happen, because all those things can be described by scalar components, which can themselves be added and scaled.

So let's consider something way more abstract. It's also commonplace to define addition for functions (forget about our previous use of  $\mathbf{f}$ ):

$$\mathbf{h} = \mathbf{f} + \mathbf{g}$$

The sum of two functions is another function, one whose value is the sum of the values of the other two functions for the same input:

$$\mathbf{h}(x) = \mathbf{f}(x) + \mathbf{g}(x)$$

And similarly we can scale a function, to make another function:

$$\mathbf{h} = k\mathbf{f}$$

$$\mathbf{h}(x) = k\mathbf{f}(x)$$

If we encounter an operator  $\hat{O}$  that somehow acts on a function to produce another function, we can ask if  $\hat{O}$  is linear. That is:

$$\hat{O}(\mathbf{f} + \mathbf{g}) = \hat{O}(\mathbf{f}) + \hat{O}(\mathbf{g})$$

is true, as is:

$$\hat{O}(k\mathbf{f}) = k\hat{O}(\mathbf{f})$$

Note that an operator is not restricted to mappings that perform arithmetic on parameters. An operator may dig into the *definition* of a function and transform

it through analysis (in coding terms, an operator can read the source of the input function, not merely call it.)

So an example of an operator would be differentiation. A function such as  $\sin$  can be differentiated analytically and the result is  $\cos$ . If we differentiate  $\cos$  we get  $-\sin$ . It doesn't matter if we:

- add the functions, then differentiate, or
- differentiate the functions, then add

Either way, we end up with  $\cos - \sin$ . This is true whatever functions we're adding, because differentiation works on each term individually and then adds the results.

The same goes for scaling, because when you amplify a function, you amplify the slope of the function.

Of course, by scaling a function we mean multiplying it by a *constant*; if we multiplied  $f(x)$  by another function  $g(x)$ , the gradient curve could end up with a wildly different shape. If we differentiate  $f(x)$  and then multiply it by  $g(x)$ , we've skipped the differentiation of  $g$ .

So, the "differentiation operator" meets the requirements of linearity, so differentiation is linear (and intuitively as integration is the inverse operation of differentiation, it too must be linear).

Another example is the Fourier transform,  $\mathcal{F}$  (§8). If you add two waves and take the Fourier transform of the combined wave, you get the same frequency distribution as if you took the Fourier transform of each wave separately and then added the two frequency distributions:

$$\mathcal{F}(\mathbf{g} + \mathbf{h}) = \mathcal{F}(\mathbf{g}) + \mathcal{F}(\mathbf{h})$$

And unsurprisingly, it's the same story with scaling:

$$\mathcal{F}(k\mathbf{g}) = k\mathcal{F}(\mathbf{g})$$

(And the same for  $\mathcal{F}^{-1}$  as you'd expect.)

This next one is a little looser as an analogy. We can classify all objects in a binary way, dividing them into members and non-members of some set. Suppose we come up with a sense in which we can add two members of the set, or scale them. Is the result always a member of the set also? If so, that's a kind of linearity.

For example, if two functions are solutions to the Schrödinger equation with some potential, they may be scaled and added to produce a third solution, so we say the Schrödinger equation is linear.

## Chapter 2

# Summation, Indices and Matrices

### 2.1 Indices

An index (plural: indices) is a subscript (and in some contexts a superscript) that stands for an integer.

$$a_n$$

This tells us that  $a$  is not just one value, but several. The  $n$  can be assumed to take a small range of values such as 1, 2, 3, the exact size of this range depending on the situation. (In physics if we have a function of integers it's usually written as a set with an index like this, with  $f(x)$  reserved for functions of continuous values.)

Instead of labelling spatial coordinates  $x, y, z$ , we can call them  $x_1, x_2, x_3$  and avoid the need to repeat ourselves by just giving the rule for the behaviour of  $x_n$ , which is then unambiguously the same for all three dimensions of space.

Often we want to add the values:

$$x_1 + x_2 + x_3 + \cdots + x_n$$

The shorthand for this is to use the  $\Sigma$  symbol:

$$\sum_n x_n = x_1 + x_2 + x_3 + \cdots + x_n$$



Later this will become so commonplace that we'll adopt an even shorter shorthand.

## 2.2 Vectors and Matrices

Thinking initially of vectors as mere collections of numbers (a viewpoint which we will rethink in §3), indices give us a way to talk about them.  $x_n$  could represent a single row or column of  $n$  numbers.

Likewise we can use two indices to label the numbers in a grid or matrix (plural: matrices). Given:

$$M = \begin{bmatrix} 5 & 2 & 7 \\ 0 & 1 & 0 \\ 4 & 6 & 8 \end{bmatrix}$$

We can refer to the elements of  $M$  as  $M_{ij}$ , with  $i$  giving the row and  $j$  the column. So:

$$M_{32} = 6$$

This unfortunately looks a lot like the number 32. When it's clear we aren't talking about raising numbers to powers, we use a combination of subscript and superscript indices, with superscripts meaning rows and subscripts meaning columns:

$$M_2^3 = 6$$

## 2.3 Matrix multiplication

If we're multiplying  $A$  and  $B$  to get  $C$ :

$$C = AB$$

in summation notation we can define the cell at row  $i$  and column  $j$  of  $C$  as follows:

$$C_j^i = \sum_k A_k^i B_j^k$$

Supposing these are square  $3 \times 3$  matrices, so all the  $i$ ,  $j$  and  $k$  can take the values 1, 2, 3. Writing out the summation for all values of  $k$ :

$$C_j^i = A_1^i B_j^1 + A_2^i B_j^2 + A_3^i B_j^3$$

This turns out to be merely one combination of some more basic operations we'll return to in §4.

## 2.4 Kronecker Delta

This is a compact way of referring to the identity matrix in summations. The diagonal elements are 1, all others are zero, which is awkward to represent in a stretchy way:

$$\hat{I} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

So instead we define the Kronecker delta, which has two indices representing row and column (the order is not important due to the symmetry of the identity matrix):

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

## Chapter 3

# Vectors

When visualising vectors as arrows, always think of them as being rooted in one spot.

When in physics we speak of a "vector field", that is, a vector at each point in space, such as wind speed and direction, or the electric field, we visualise arrows spread out over space. But the value of the field in two different places may be the same.

This is obvious (and less confusing) in the case of a scalar field, such as temperature. At two different locations in a room, the temperature may be the same. It's a numerical value that varies from place to place, and the same number may appear in two places.

But exactly the same is true for a vector field. If the wind is some particular speed and direction at two different places on the map, we say the vectors are equal: they are the *same vector*. It is irrelevant that they are associated with different locations in physical space. In vector space, there is one vector with that direction and length.

### 3.1 Vectors as geometric objects

What is a two dimensional vector? A common starting point is to say it's two numbers, and we very often casually refer to a column like this as a vector:

$$\begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

But for the purposes of physics, vectors are primarily geometric objects. They can be described with numeric coordinates, but there is no preferred coordinate basis.

To understand what we are giving up, it may help to initially visualise the space of plane vectors as having some intrinsic coordinate grid built into it, so every vector in that space "knows" its own numeric coordinates, being fixed to that grid.

But to think about vectors in an abstract way, it's best not to assume anything about their nature except that they meet the requirements of a vector space.

For some unknown vector space that we assert to be two dimensional, a pair of numbers only describes a vector if we have a basis  $[\vec{e}_1 \quad \vec{e}_2]$  to multiply by:

$$[\vec{e}_1 \quad \vec{e}_2] \begin{bmatrix} 3 \\ 2 \end{bmatrix} = 3\vec{e}_1 + 2\vec{e}_2$$

A property of a vector is that you can multiply it by a scalar to get another vector (unless you multiply by 1, in which case you get the same vector), and another property is that you can add two vectors (placing them end to end) to get another vector. So an expression such as:

$$3\vec{e}_1 + 2\vec{e}_2$$

describes a new vector that we have produced by mixing together two basis vectors. Any vector in the space can be described in this way. And therefore any vector can be decomposed into coordinates, but only once you have chosen some basis vectors.

It's not necessarily possible to say anything numerically about a single vector, because it can't be described numerically without introducing basis vectors to measure it against. A vector has a length and a direction, but these things can only be measured in relation to other vectors.

A vector space is a set of vectors, and we can if we like think of the vectors in the space as having an absolute existence, but we cannot say that there is one correct perspective to view those vectors from, any more than we can assume the North Pole is the "top" of the Earth, nor one correct scale to measure them by.

All we can say is that there is some angle between two vectors, or some ratio between the lengths of two vectors.

It follows that we cannot meaningfully communicate our choice of basis to anyone in terms of that basis alone. The coordinates of our two chosen basis vectors, if we express them in terms of our basis itself, are always:

$$e_1 = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

$$e_2 = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

That is,  $\vec{e}_1$  contains 1 unit of itself and nothing of  $\vec{e}_2$ , and the reverse situation for  $\vec{e}_2$ . This is like saying "it is what it is." It looks like the identity matrix (this is not a coincidence):

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The realisation of this relativistic nature of vectors can produce confusion, just as may occur when we first encounter the idea that position in physical space is not absolute, velocity is not absolute, etc. It just has to be accepted. But we can suppose the existence of an intrinsic hidden absolute basis, a coordinate grid, and use this as a mental crutch to stabilise ourselves, while gradually developing an understanding that this crutch is not necessary.

The question remains: how do we identify a set of basis vectors? If we have an inner product then we can pick an orthonormal basis, because we can make sure each basis vector is of unit length (inner product with self is 1) and all are mutually orthogonal (inner product is 0).

## 3.2 Vector Spaces

If vectors are not merely collections of numbers it's important to be clear what they are. A vector space is a set of objects that meet certain abstract criteria. As soon as we can identify a way of meeting all the criteria, the set of objects is a vector space and the objects are vectors.

It may be worth throwing out any preconceptions about vectors based on picturing arrows drawn on grid paper and just say that there is a set of mysterious "objects" of which we will state some abstract properties, but leave anything else unspecified.

### 3.2.1 They can be added

There is an operator  $+$  that takes two objects from the set and returns another from the same set (so it's a closed operator).

This operator is commutative:

$$\vec{u} + \vec{v} = \vec{v} + \vec{u}$$

and associative:

$$\vec{u} + (\vec{v} + \vec{w}) = (\vec{v} + \vec{u}) + \vec{w}$$

There is a special object called 0, which makes no difference when added to any object from the set:

$$\vec{v} + 0 = \vec{v}$$

Also every object has an opposite, known as its additive inverse, so they pair up. The inverse of  $\vec{v}$  is written as  $-\vec{v}$ , and:

$$\vec{v} + (-\vec{v}) = 0$$

The above can be written as  $\vec{v} - \vec{v}$ .

### 3.2.2 They can be scaled

There is an associated set of objects called scalars, typically restricted to real or complex numbers. Our objects can be multiplied by a scalar to get another object. Scaling them by 1 makes no difference. Scaling them by  $-1$  discovers the additive inverse.

Given two scalars  $a$  and  $b$ , we can compute  $c = ab$  and then scale an object  $\vec{v}$  by it, or we can separately scale the object first by  $a$  and then by  $b$ , and the result is the same:

$$(ab)\vec{v} = a(b\vec{v})$$

Scaling is distributive over addition of objects:

$$a(\vec{u} + \vec{v}) = a\vec{u} + a\vec{v}$$

And also over addition of scalars:

$$(a + b)\vec{v} = a\vec{v} + b\vec{v}$$

### 3.2.3 The Field

A vector space's set of scalars is known as its field. It can be any sort of object for which we can define addition, subtraction, multiplication and division, so real or complex numbers usually serve this purpose, but there exist vectors that cannot serve as a field of scalars for other vector spaces. For example, familiar geometric vectors cannot be multiplied and divided in a way that is closed.

### 3.2.4 Examples of Vector Spaces

Any set of objects for which we can define these operations is a vector space. This means that the real numbers  $\mathbb{R}$  and complex numbers  $\mathbb{C}$  themselves qualify as vector spaces.

Ordered pairs of real numbers,  $\mathbb{R}^2$ , clearly also qualify, because addition can add the first and second pair members separately, scaling can scale both of the members, and then all the other requirements follow automatically.

### 3.3 Dot Product

Also known as the scalar product (an exact synonym), sometimes as "the inner product" (not an exact synonym, as we'll see).

The dot product is a scalar-valued operator between two vectors,  $\vec{p} \cdot \vec{q}$ . It has the same scalar value under a change of coordinate system, as long as the basis vectors remain the same length and orthogonal (i.e. under rotation or reflection).

If the two vectors  $\vec{p}$  and  $\vec{q}$  are separated by angle  $\theta$ , and we know the magnitude (length) of each vector, e.g.  $\|\vec{p}\|$ , then

$$\vec{p} \cdot \vec{q} = \|\vec{p}\| \|\vec{q}\| \cos \theta$$

Aside from the immediately obvious fact that it is commutative (swapping the vectors makes no difference), the behaviour of  $\cos$  has some implications.

First, as  $\cos 0 = 1$ , for vectors pointing in the same direction we just multiply their magnitudes. Further, the dot product of a vector with itself is the square of the magnitude:

$$\vec{p} \cdot \vec{p} = \|\vec{p}\|^2$$

And of course if it's a unit vector, the result is  $1^2 = 1$ .

Second, as  $\cos \pi = -1$ , for vectors pointing in opposite directions, the result is the same but negative:  $-\|\vec{p}\| \|\vec{q}\|$ .

Third, as  $\cos(\pi/2) = \cos(3\pi/2) = 0$  orthogonal vectors have dot product equal to zero. So given a Euclidean basis (a set of orthonormal basis vectors)  $\vec{e}_n$ :

$$\vec{e}_i \cdot \vec{e}_j = \delta_{ij}$$

Note that this is an observation about a set of orthonormal vectors, so even though we've used indices to label directions, we aren't talking about coordinates *yet*.

### 3.3.1 Finding coordinates

It's also interesting to consider the dot product of any vector  $\vec{p}$  with a unit vector, such might make a suitable basis vector  $\vec{e}_n$ . If  $\vec{p}$  is in the same direction as  $\vec{e}_n$ , the dot product is just  $\|\vec{p}\|$ . If orthogonal, it's zero.

For angles between, consider the right triangle, where:

$$\cos \theta = \frac{\text{adjacent}}{\text{hypotenuse}}$$

So if the hypotenuse is our vector  $\vec{p}$ , hence of length  $\|\vec{p}\|$  and the side adjacent to  $\theta$  is a vector in the same direction as one of our unit basis vectors  $\vec{e}_n$  scaled by some factor we will call  $p_n$ , which is therefore the magnitude of that vector and the length of the adjacent side:

$$\cos \theta = \frac{p_n}{\|\vec{p}\|}$$

Then:

$$\vec{p} \cdot \vec{e}_n = \|\vec{p}\| \|\vec{e}_n\| \cos \theta = \|\vec{p}\| \|\vec{e}_n\| \frac{p_n}{\|\vec{p}\|} = \|\vec{e}_n\| p_n$$

But  $\vec{e}_n$  is a unit vector so  $\|\vec{e}_n\|$  is 1, and therefore:

$$\vec{p} \cdot \vec{e}_n = p_n$$

So it is the *projection* of  $\vec{p}$  on to  $\vec{e}_n$ , which is to say it is the  $n$ -th coordinate,  $p_n$  of  $\vec{p}$ . Thus we can reconstitute  $\vec{p}$  by summation:

$$\vec{p} = \sum_n \vec{e}_n p_n = \sum_n \vec{e}_n (\vec{p} \cdot \vec{e}_n)$$

That is,  $\vec{p}$  is the sum of its component vectors, each of which is a basis vector scaled by a coordinate, that coordinate being the result of the dot product between  $\vec{p}$  and the basis vector.

### 3.3.2 Dot Product is Homogeneous

Intuitively, a triangle scales linearly. If the hypotenuse is scaled by some factor  $k$ , the adjacent side will also scale by  $k$ :

$$k(\vec{p} \cdot \vec{e}_n) = (k\vec{p}) \cdot \vec{e}_n$$

So the dot product is *homogeneous*.



### 3.3.3 Dot Product is Distributive

Vector addition also has a useful simplifying property. Consider two vectors  $\vec{q}$  and  $\vec{r}$ . Each has a component along basis vector  $\vec{e}_n$ , so:

$$\vec{q} \cdot \vec{e}_n = q_n$$

$$\vec{r} \cdot \vec{e}_n = r_n$$

If we picture  $\vec{q}$  and  $\vec{r}$  laid head to tail, the total distance travelled in the direction of  $\vec{e}_n$  is  $q_n + r_n$ , or:

$$\vec{p} \cdot (\vec{q} + \vec{r}) = \vec{p} \cdot \vec{q} + \vec{p} \cdot \vec{r}$$

This means the dot product is *distributive* over vector addition.

### 3.3.4 Do not interchange scalar and dot product

It may be worth drawing attention to a tempting manipulation that is not valid:

$$\vec{p}(\vec{q} \cdot \vec{r}) \neq \vec{q}(\vec{p} \cdot \vec{r})$$

Each side multiplies either  $\vec{p}$  or  $\vec{q}$  by a scalar. It doesn't matter that the scalar is obtained from the dot product; it's just a scalar. Multiplying a vector by a scalar will not change its direction, so there is no reason the results will be in the same direction.

## 3.4 Using coordinates

Having done the hard work (computing  $\cos$ ) in order to obtain the coordinates, things subsequently become much easier. Given a basis  $\vec{e}_n$  and a pair of vectors,  $\vec{p}$  and  $\vec{q}$ , with coordinates  $p_n$  and  $q_n$ , so:

$$\vec{p} = \sum_n \vec{e}_n p_n$$

$$\vec{q} = \sum_n \vec{e}_n q_n$$

For the dot product, using the coordinate form of  $\vec{p}$ :

$$\vec{p} \cdot \vec{q} = \left[ \sum_n \vec{e}_n p_n \right] \cdot \vec{q}$$

As the dot product is distributive over addition, that means we can move it inside the summation:

$$\vec{p} \cdot \vec{q} = \sum_n [\vec{e}_n p_n \cdot \vec{q}]$$

And because it is homogeneous, we can gather the vectors:

$$\vec{p} \cdot \vec{q} = \sum_n p_n [\vec{q} \cdot \vec{e}_n]$$

But  $\vec{q} \cdot \vec{e}_n$  is the projection of  $\vec{q}$  on to  $\vec{e}_n$ , that is, it is the coordinate  $q_n$  of  $\vec{q}$  in the direction of  $\vec{e}_n$ , so:

$$\vec{p} \cdot \vec{q} = \sum_n p_n q_n$$

And so for two vectors expressed as coordinates in a common basis, we just multiply their corresponding coordinates and sum the results, which is ridiculously simple (no cos at all), and which is why the coordinate approach is so attractive for calculation.

In the case where  $\vec{p} = \vec{q}$ :

$$\vec{p} \cdot \vec{p} = \sum_j p_j^2$$

Which is Pythagorus's theorem, agreeing with our earlier claim that the dot product of a vector with itself is the square of the magnitude.

### 3.5 Change of Basis

A matrix can be used to:

- map vectors to a new length and direction in the same basis, or
- perform a coordinate conversion on vectors so they remain the same vectors but expressed in different numerical coordinates.

The mathematical machinery is identical.

Viewed as an operator, the matrix may have eigenvectors only in some directions. The operator is therefore a geometrical object just as a vector is, and the matrix elements may be numerically different depending on the basis, just as the coordinates of a vector may differ depending on the basis, despite describing the very same objects regardless of the basis chosen.

Viewed as a coordinate converter, the matrix effectively depends on two bases, the one being converted from and the one being converted to.

### 3.5.1 Effect of change of basis on vectors

A plane vector  $\vec{v}$  in some basis can be expressed in coordinates as a column matrix  $V$ :

$$V = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

And with the basis as a row matrix:

$$E = [\vec{e}_1 \quad \vec{e}_2]$$

Matrix multiplication builds the vector:

$$\vec{v} = EV = 3\vec{e}_1 + 4\vec{e}_2$$

We can create a matrix that will double the length of the basis vectors:

$$G = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

By the rules of matrix multiplication the bases needs to be on the left:

$$E' = EG = [2\vec{e}_1 \quad 2\vec{e}_2]$$

What coordinates would  $\vec{v}$  have in this new basis  $E'$ ? Intuitively the coordinates need to be halved to refer to the same vector. So we need the inverse of  $G$ , written as  $G^{-1}$ , which shrinks the coordinates, so we'll call it:

$$S = G^{-1} = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$$

And so our vector's coordinates become:

$$V' = SV = \begin{bmatrix} 1.5 \\ 2 \end{bmatrix}$$

This is the same vector as before, just in different coordinates:

$$\vec{v} = EV = E'V'$$

We say that vectors are *contravariant* under a change of basis.

### 3.5.2 Dot product under change of basis

The dot product depends on the lengths of two vectors and the angle between them. If the vectors are represented as coordinates in some basis, then a change of basis will change the coordinates. Will the dot product change too? It depends.

If the basis vectors are only rotated or reflected, this preserves both lengths and angles, so the dot product will be unaffected.

If the basis vectors are scaled, the lengths implied by the coords will change and so the dot product will change. To take the above example, we grow the basis vectors with  $G$ , having the equivalent effect on the coordinates to shrinking the input vectors with  $S$  to half their original length, and so the dot product will be  $\frac{1}{4}$  of its original value.

If the basis vectors are skewed, this will have the equivalent effect on the coordinates of skewing the input vectors, changing the angle between them.

## 3.6 Covectors

A covector is a scalar-valued linear function of a vector that performs the dot product using a pre-determined other vector.

$$f_n(\vec{v}) = \vec{e}_n \cdot \vec{v}$$

In other words, every vector has a corresponding covector which extracts a coordinate along the direction of that vector.

It can be expressed as a row matrix with scalar components. For example the coordinates of a basis vector  $\vec{e}_n$  could be written as a row matrix:

$$E_n = [1 \quad 0]$$

This is a covector, distinguished by being a row rather than a column. So to apply the covector is just matrix multiplication:

$$E_n V$$

where  $V$  is the column matrix of the coordinates of the input vector  $\vec{v}$ .

We can construct such a function for all  $n$  basis vectors, and these form a basis in the so-called dual space of all possible covectors, which is itself a vector space, each covector being defined by only by a set coordinates.

Following the above narrative our  $\vec{v}$  is now expressed as  $V'$ , having been shrunk by  $S$  to work in basis  $E'$ . We now want evaluate  $F_n$  on  $V'$ , but there is an incompatibility of basis, because  $F_n$  has the  $n$ -th basis vector of  $E$  in its definition.

Or to put it simply, the coordinates in  $V'$  have been shrunk, whereas  $F_n$  only works correctly with unshrunk coordinates.

We can fix this by pre-converting the input vector:

$$E_n G V$$

This new covector applies matrix  $G$  to the input, growing it so it becomes compatible with  $E_n$ . But as can be easily verified, it makes no difference to the result whether we evaluate  $GV$  or  $E_n G$  first; this is the beauty of linear functions. Thus we can produce an amended row-matrix based on the original:

$$E'_n = E_n G$$

It has a built-in "growth factor", and so is compatible with vectors that have been shrunk.

This means that under a change of coordinate systems, where the basis vectors have had  $G$  applied to them, covectors must also have  $G$  applied to them. This is the opposite of what has to happen to vectors.

As a result we say covectors are *covariant* (this is the source of the name covector).

### 3.7 Operators

An operator  $\hat{O}$  is a function that maps from vectors to vectors. That is, the input is a vector and so is the output. It may change the length or direction of the vector.

We are particularly interested in linear operators, for which:

$$\hat{O}(x\vec{i} + y\vec{j}) = x\hat{O}\vec{i} + y\hat{O}\vec{j}$$

Why? Because if you have chosen your basis  $\vec{i}, \vec{j}$  and so you can express all vectors in coordinates  $(x, y)$ , i.e. as simple "weighted sums" of your two basis vectors,  $x\vec{i} + y\vec{j}$ , then to apply  $\hat{O}$  to a vector, all you need to know is  $\hat{O}\vec{i}$  and  $\hat{O}\vec{j}$ .

By applying the operator to the basis vectors, you discover two new basis vectors:

$$\vec{i}' = \hat{O}\vec{i}$$

$$\vec{j}' = \hat{O}\vec{j}$$

The coordinates you would use to express an input vector:

$$\vec{v} = x\vec{i} + y\vec{j}$$

can be used to mix these new basis vectors and get the result of applying the operator to the input vector:

$$\hat{O}\vec{v} = \hat{O}(x\vec{i} + y\vec{j}) = x\vec{i}' + y\vec{j}'$$

A matrix can be interpreted as a way to convert coordinate vectors from one basis to another, preserving the same meaning, or as a way to produce a different vector in the same basis.

Considering the latter use, i.e. linear operators that transform vectors, what effect does a change of basis have on vector coordinates?

### 3.8 Eigenvectors and Eigenvalues

An operator that performs only scaling (e.g.  $G$  and  $S$ ) is isotropic, treating all directions equivalently.

But some operators are biased with regard to direction. To characterise the behaviour of an operator we can consider those vectors which are scaled by it without their direction being altered (the scaling may be negative, leaving the vector pointing the opposite direction; as long as the resulting vector is co-linear with the input vector, that's insignificant enough.) Such vectors are called the *eigenvectors* of the operator, and the corresponding scalar values are the *eigenvalues*.

So in the case of  $S$  and  $G$ , all input vectors are eigenvectors: all inputs get only scaled, and always by the same eigenvalue.

With vectors in the plane, when the operator is a pure rotation, e.g. by a right-angle anti-clockwise:

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

or clockwise:

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

every vector changes direction by the same angle, and that means there are no eigenvectors.

The zero vector is not considered a candidate for an eigenvector; regardless of the operator, it goes from length zero to length zero, so any scalar could be the eigenvalue, meaning that the eigenvalue is undefined.

In three dimensions the rotation has an axis, along which all vectors are eigenvectors. Curiously, even though these vectors don't exist in the plane, we can find *complex* eigenvalues for them by supposing that such eigenvectors exist, which is weird.

More interestingly, there are operators for which only some vectors are eigenvectors. Consider a reflection (call it  $M$  for mirror):

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

If we take the first coordinate to be horizontal and the second vertical, this flips the input vector to point up rather than down, or vice versa. So it seems that all vectors have their direction changed and are not eigenvectors, but there are exceptions: vectors that lie on the horizontal axis and have no vertical component will be unaffected, i.e. they will be eigenvectors with eigenvalue 1. Also vectors that lie on the vertical axis will have their direction changed, but to the exact opposite direction, which is the same as being scaled by -1, and so these too are eigenvectors, but with eigenvalue -1.

So within the space of input vectors, there is a subspace (the *eigenspace*) of eigenvectors, and  $M$  has an intrinsic orientation, as there is a particular line around which reflection occurs.

We can find the eigenvectors given a matrix representation  $M$  of an operator acting on a vector represented by a column matrix  $v$ . If  $v$  is an eigenvector, and  $x$  is the corresponding eigenvalue, what we mean by that is:

$$Mv = xv$$

For the vector  $v$ , multiplying it by the matrix  $M$  is the same as multiplying it by the ordinary number  $x$ . So with trivial algebra:

$$Mv - xv = 0$$

This is fine because  $Mv$  and  $xv$  are column matrices, and here 0 is the column matrix filled with zeros.

Pulling out  $v$  as a factor (not quite as trivial):

$$(M - xI)v = 0$$

We have to leave behind the identity matrix  $I$  in place of  $v$  because we need the matrix equivalent of the ordinary number  $x$ , so we can subtract it from  $M$ .

Having split it into two factors whose product is zero, we know that either one or both of the factors must be zero. We already realised we aren't interested in the case where  $v$  is the zero vector because its eigenvalue will be undefined (it could be anything). So we refuse to accept 0 as an eigenvector. Therefore  $v$  is not the zero vector, and so the matrix  $M - xI$  must be such that it is able to transform some non-zero vector  $v$  into the zero vector. This means it has no inverse, as there is no way to recover the direction of the original vector if we've sent it to 0 (the zero vector has no direction, or has all directions, so direction is a meaningless concept for it.)

One way to picture the effect of a matrix is to think of it acting on a unit square (where the matrix is  $2 \times 2$ ) and asking what the area of the resulting parallelogram will be. If it is not zero, every point in the original square has a unique point in the parallelogram and vice versa: the matrix is invertible. If the area is zero, the points of the original square have been crammed onto a line of 1 dimension, so we have destroyed the information about where they came from in 2 dimensions. All input vectors end up pointing in the same direction, and are only distinguished by length. No linear transform will be able to spread them back out into the correct different directions: the matrix is not invertible.

The area of that parallelogram (or in higher dimensions, the volume of an  $n$ -parallelepiped) is called the determinant of the matrix,  $\det M$ . If it's zero, the matrix is not invertible. And therefore, if:

$$\det(M - xI) = 0$$

then we definitely have some eigenvalues. The determinant can be expanded out into a polynomial expression in  $x$  (there are various methods; a popular one is to get a computer to do it) and then solved by factoring to find all the  $x$  values that make one of the factors 0. We can then plug those  $x$  values back into:

$$(M - xI)v = 0$$

one at a time, and solve to find the corresponding  $v$ . Thankfully all this can be mechanised.



### 3.9 Symmetric Matrices

One interesting kind of operator is any represented by a symmetric matrix in some basis, so  $M^T = M$ , or  $M_{ij} = M_{ji}$  for all combinations of  $i$  and  $j$ . So the diagonal elements are unconstrained, but all others have to match their diagonally-opposite element.

The curious thing about them is that their eigenvectors are orthogonal and completely span the vector space. That is, in an  $N$  dimensional space, they perform a scaling in all  $N$  available orthogonal directions, stretching or squishing.

This means that if you find the eigenvectors of the operator, you've found an orthogonal basis. This is hugely important in Quantum Mechanics (§9), albeit with some modifications for complex numbers.

### 3.10 Effect of Change of Basis on Operator

If we apply  $R_A$  to our two basis vectors, all our non-zero vectors' coordinates will need to change (while still being the same vectors, of course, just expressed in a new basis.) This means, just as we had to fix our covector, we now need to come up with the matrix  $M'$  that mirrors around the same line as  $M$  did in the un-rotated basis. We say that  $M'$  and  $M$  represent the same operator in different coordinate systems.

This time it will be a three step process:

- adjust the input vector so it is expressed in  $M$ -compatible ("pre-rotation") coordinates
- apply  $M$  to the pre-rotation coordinates, to get the reflected vector in pre-rotation coordinates
- adjust the reflected vector into post-rotation coordinates

As we applied  $R_A$  to the basis vectors, that means we must have applied  $R_C$  to all the column matrices representing our vectors in coordinate form (clockwise rotation being the inverse of anti-clockwise rotation). So the three steps appear to the left of our input  $V$ :

$$M'V = R_C M R_A V$$

In English, reading from the right, take the input  $V$ , rotate it anti-clockwise (to undo the clockwise rotation we assume has been performed on it), then apply the original  $M$  matrix for reflection, then rotate clockwise.

As with the covector example, we can ditch the example input  $V$  and just compute the matrix by itself for later use with any  $V$ :

$$M' = R_C M R_A$$

So the matrix  $M'$  represents the same operator as  $M$  in the anti-clockwise rotated coordinate system.

When it comes to classifying this as covariant or contravariant, we have a puzzle. It was necessary to perform both kinds of coordinate transformation here.

There is a general pattern to these examples, vectors, covectors and operators, which is captured in the notion of a tensor.

### 3.11 Inner Product

An inner product is a scalar-valued operator between two vectors:

$$\langle \vec{p}, \vec{q} \rangle$$

A vector space equipped with such an operator is called an *inner product space*. The most well known example is the dot product. To qualify as an inner product an operator must satisfy certain properties. It must be commutative:

$$\langle \vec{p}, \vec{q} \rangle = \langle \vec{q}, \vec{p} \rangle$$

This is obviously true for the dot product as we simply multiply matched components and then sum them. Denoting the  $i$ -th component by  $p_i$  and  $q_i$ :

$$\sum_i p_i q_i = \sum_i q_i p_i$$

We also require:

$$\langle \vec{p} + \vec{r}, \vec{q} \rangle = \langle \vec{p}, \vec{q} \rangle + \langle \vec{r}, \vec{q} \rangle$$

Again this is obviously true as it's just multiplying out each term of the summation:

$$\sum_i (p_i + r_i) q_i = \sum_i p_i q_i + r_i q_i$$

The inner product notation is simply telling what is true of each term.

The next requirement ( $\alpha$  being some scalar constant) is therefore no surprise:

$$\langle \alpha \vec{p}, \vec{q} \rangle = \langle \vec{p}, \alpha \vec{q} \rangle = \alpha \langle \vec{p}, \vec{q} \rangle$$

and so we are always just summing the product  $\alpha p_i q_i$  and the order makes no difference to the result.

There are further requirements that are discarded in some contexts:

$$\langle \vec{p}, \vec{p} \rangle \geq 0$$

For the Euclidean dot product we're squaring the coordinates  $p_i$  so the result must be positive. But in Relativity (§10) we allow negative ("spacelike") intervals, which is why this requirement is not always applied.

Finally,  $\langle \vec{p}, \vec{p} \rangle = 0$  if and only if  $\vec{p}$  is the zero vector. Again this could be untrue in Relativity if the time and space contributions cancel out ("lightlike").

Generalising on the dot product, we can introduce a second summation index  $j$  and make all the combinations  $p_i q_j$ , and then decide how much of a contribution to the sum each combination should make by controlling it with a matrix  $A_j^i$  and now per Einstein we can say:

$$p_i A_j^i q^j$$

Which is equivalent to putting the transpose of  $\vec{p}$  on the left, the matrix  $\mathbf{A}$  in the middle and  $\vec{q}$  on the right and doing matrix multiplication (and it doesn't matter how we group the operations):

$$\vec{p}^T \mathbf{A} \vec{q}$$

Indeed, the above requirements on an inner product effectively mean that any inner product must be expressible in this form.

In the standard dot product, we are only interested in the diagonal combinations,  $p_i q_j$  where  $i = j$ , but this is equivalent to saying that  $\mathbf{A}$  is the identity matrix  $\delta$ .

This idea is generalised further when considering complex vector spaces.

### 3.12 Complex vector spaces

Any vector space is defined over a *field*. This is unrelated to the physics meaning of "field", a value defined at each point in a space. Here a field is any set of objects with binary operators for addition, subtraction, multiplication and division that behave like those of the real numbers, so  $\mathbb{R}$  is a field.

But as complex numbers meet this criterion therefore  $\mathbb{C}$  is also a field, and therefore a vector space may be complex, and have complex coordinates.

Even the simplest non-trivial example,  $\mathbb{C}^2$ , is not directly imaginable, because although each vector requires two coordinates, each of those is a complex number incorporating a real and imaginary part, so each vector requires four real numbers to describe it, and so  $\mathbb{C}^2$  can be mapped to  $\mathbb{R}^4$ , which is impossible to visualise directly.

Even so, concepts applicable to real vector spaces also work for complex, although with some modifications. The main issue is determining the modulus, for which we must introduce an inner product.

If we use the usual dot product definition then we have a problem because we naturally expect the modulus to be a positive real number. Summing the squares of the components of a complex vector could well produce a negative result, and then we need to take the square root to get the modulus, so the modulus wouldn't even be a real number.

To ensure  $\langle \vec{u}, \vec{v} \rangle$  is real and positive, we amend the inner product so that we first take the complex conjugate of one its arguments:

$$\langle \vec{u}, \vec{v} \rangle = \vec{u}^* \cdot \vec{v}$$

This has the complicating side-effect that commutativity:

$$\langle \vec{u}, \vec{v} \rangle = \langle \vec{v}, \vec{u} \rangle$$

no longer applies. But who says it needs to? We instead make the requirement be:

$$\langle \vec{u}, \vec{v} \rangle = [\langle \vec{v}, \vec{u} \rangle]^*$$

This is sometimes called conjugate symmetry. If all the components are real then complex conjugation makes no difference and commutativity is restored, so the nice thing is that we've amended the rule in a way that is "backward compatible" with real vectors.

This does mean that when taking the inner product of two different complex vectors, it matters which one we take the complex conjugate of. In physics the convention is to take the conjugate of the LHS vector.

The general form of the inner product, where we supply a matrix to control how to pair up and weight the coordinates, is similarly amended.

We use the dagger  $^\dagger$  symbol to mean conjugate transpose, where we transpose a matrix (so turn a column vector into a row) and also take the complex conjugate of every element. It's equivalent to applying both  $^\top$  and  $^*$ .

$$\langle \vec{u}, \vec{v} \rangle = u^\dagger \mathbf{M} v$$

As usual if  $\mathbf{M}$  is  $\delta$  then this reduces to the first definition given above. It should at least be self-adjoint or Hermitian, which is to say that:

$$\mathbf{M}^\dagger = \mathbf{M}$$

That is, every element is the complex conjugate of its diagonally opposing element, and that therefore elements on the diagonal are real (they aren't moved by the transposition and so must equal their own complex conjugates).

A matrix like this is the complex equivalent of the real symmetric matrix for which we gave a definition (§3.9).

Several other important facts about Hermitian operators can be derived: their eigenvalues are all real, their eigenvectors are orthogonal and span the space and so can be used to construct an orthonormal basis.

Another interesting kind of operator in complex spaces is those where:

$$\mathbf{U}^\dagger \mathbf{U} = I$$

i.e. the identity operator. These are known as unitary operators. They have the property of preserving the inner product (which is the same property we observed before for rotations and mirrorings):

$$\langle \vec{u}, \vec{v} \rangle = \langle \mathbf{U}\vec{u}, \mathbf{U}\vec{v} \rangle$$

If you have a Hermitian operator expressed by the matrix  $M$  you can convert it to another representation by wrapping it in a transformation  $T$  and its inverse:

$$M' = TMT^{-1}$$

If  $T$  is unitary then  $M'$  will be Hermitian, recognisable by the relationship between diagonally opposite matrix elements.

## Chapter 4

# Tensors

### 4.1 Einstein Notation

Where we sum over terms where the summation variable (in this case  $n$ ) appears twice, once as superscript and once as subscript, which happens a lot, Einstein got tired of writing the summation symbol so many times and so adopted the convention of omitting it:

$$C_j^i = A_n^i B_j^n$$

Note that where we apply this to transformations on a geometric space, the number of dimensions determines the range of every loop variable. So in 3 dimensions,  $i$ ,  $j$  and  $n$  are all  $\in 1, 2, 3$ .

Also bear in mind that the distinction between subscript and superscript indices is going to be important, and in Einstein's summation notation the repeated variable in a term must appear once as a subscript and once as a superscript index, as will become clear later on.

The summation loop variable  $n$  (known as a *bound* or *dummy* variable) is clearly different from the other two variables. We are not summing over  $i$  or  $j$ , because we are preserving separate matrix cell values  $C_j^i$  in the output, not mixing them together.

Einstein's notation always makes it unambiguous what operations we are performing. if there are no repeated indices, there is no summation: we're doing the tensor product.

$$C_j^i = A^i B_j$$

This literally just tells us how to compute the element  $(i, j)$  of  $C$ , by multiplying the  $i$ -th element of  $A$  and the  $j$ -th element of  $B$ .

If there is at least one repeated element, we're doing contraction, i.e. summation:

$$E^i = C_j^i D^j$$

This is telling us how to compute the  $i$ -th element of  $E$ , by summing over  $j$  the element  $(i, j)$  of  $C$  multiplied by the  $j$ -th element of  $D$ .

So there's never any ambiguity, but also it's not necessary to say whether you're doing the tensor product or contraction.

## 4.2 Tensor Product

Suppose rather than a square matrix, we had a cubic lattice, and thus needed three loop variables,  $i, j, k$  to address each element. We can picture this as a cube and write its elements as  $A_{ijk}$  (we have arbitrarily used subscript indices - that distinction is irrelevant here).

We can make the outer product  $\otimes$  (also known as the tensor product) between this cube and a square matrix  $B_{pq}$  by pairing up every combination of their elements and multiplying them.

$$C_{ijkpq} = A_{ijk} B_{pq}$$

This means that  $C$  is a 5-dimensional object which seems difficult to picture at first, but there is a completely obvious way to think about it: imagine a square grid addressed by  $p, q$ , and in each cell is a small cube of numbers addressed by  $i, j, k$ . So the full address of each number requires five numbers,  $p$  and  $q$  to find a grid cell and then  $i, j, k$  to locate a cell of the cube found within that grid cell. The number in each piece of a cube (and that cube sitting a grid cell) is the product of the corresponding cells in the original  $A$  cube and the  $B$  grid.

By the way, we avoid calling it 5-dimensional (even though that is an accurate description of the structure) because we already use dimension to refer to the range of each index:  $i \in 1, 2, 3$  would mean three dimensions, even though we have 5 indices like that. So we say the number of indices is the *rank* of the tensor.

Note that in geometrical tensors we are frequently only interested in index variables that are all of the same dimension: squares, cubes, and so on, because they relate to the dimensionality of the geometric space.

### 4.3 Superscript and Subscript Indices

When considering matrices (which is to say, rank-2 tensors) we think of the superscript index as the row and the subscript as the column. So a column vector's coordinates are superscripted, whereas a row vector's are subscripted. And so a matrix can be thought of as a set of column vectors side by side, or a set of row vectors stacked in layers.

This is not a meaningful rule with higher rank tensors.

In fact the true rule is that a contravariant index is superscript while a covariant index is subscript. And then the convention with matrices is that rows are covariant and columns are contravariant. This matches up with our convention of writing ordinary vectors (contravariant) as columns and covectors (covariant) as rows.

A matrix can be thought of as a stack of row vectors. Each row defines a function for extracting a coordinate from a column vector, relative to a basis vector.

We can quite happily produce a tensor product mess such as:

$$C_{jkq}^{ip} = A_{jk}^i B_q^p$$

In the tensor product, if an index is superscript in a source tensor, it remains a superscript in the output tensor, and the same for subscripts.

The various indices have each been arbitrarily thrown into one of the two available locations. In terms of the arithmetical machinery they all behave identically, but preserving these two types ensures that the resulting tensor will be transformable under a change of basis.

### 4.4 Tensor Contraction

In the tensor product there are no repeated indices in the terms so Einstein notation tells us there is no summation.

To introduce summation will mean collapsing cells together, reducing the rank of the structure. This allows us to arrive at the dot product in a roundabout, two-stage process.

If we do the tensor product on two rank-1 tensors,  $A_i$  and  $B^j$ , the result  $C_i^j$  is a rank-2 tensor (a matrix).

$$A \otimes B = C_i^j = A_i B^j$$

We've been careful here to follow a convention in assigning superscript and subscript indices so  $A_i$  is a row and  $i$  denotes the column within that row, and



$B^j$  is a column and  $j$  denotes the row within that column. We then always place the row on the left and the column on the right.

To obtain the dot product, we throw away everything but the main diagonal of that grid, all the elements where  $i = j$ , and we sum those elements. The Kroneker delta expresses this:

$$A \cdot B = \sum_i \sum_j A_i B^j \delta_{ij}$$

Or we can realise that we only need one variable, "contracting"  $i$  and  $j$  into just  $i$  alone:

$$A \cdot B = \sum_i A_i B^i$$

And as this fits the pattern of Einstein notation, we can just write:

$$A \cdot B = A_i B^i$$

Because  $i$  appears twice in the term (once each as a subscript and a superscript), this is a summation of the diagonal elements.

The result is a single scalar value, also known as a rank-0 tensor. So the above process (known as *contraction*) has reduced the rank by 2, and this in fact is what always happens regardless of the rank of the tensors involved.

The only rule is that the contraction must involve one subscript and one superscript index. The arithmetic will blindly work if this rule is broken, but the result will not have geometrical meaning.

We can arrive at matrix multiplication in the same way. If we do the tensor product on two rank-2 tensors (matrices),  $A_j^i$  and  $B_q^p$ , the result  $C_{jq}^{ip}$  is a rank-4 tensor (a grid of grids?)

$$A \otimes B = C_{jq}^{ip} = A_j^i B_q^p$$

Let's perform contraction C by replacing  $p$  with  $j$  (this is a valid thing to do because  $j$  is a subscript and  $p$  is a superscript, so they are the opposite kinds of index; we could have chosen  $i$  and  $q$  instead).

$$C_q^i = A_j^i B_q^j$$

As  $j$  is now a repeated (dummy) index, this is a summation. We're doing something similar to taking the diagonal of a matrix, and we can reorganise our visualisation  $C_{jq}^{ip}$  to something much simpler than a hypercube, via the trick of thinking about nested grids.

Picture a square grid addressed by  $i, q$ , and in each of its cells there is another grid of numbers, addressed by  $j, p$ , and those numbers are each the product  $A_j^i B_q^p$ . So when we say that  $p = j$ , we're literally taking a diagonal of each of the nested grids, to get a set of numbers  $A_j^i B_q^j$  that we sum together, so we end up with a single number in each cell of the outer grid, and it becomes merely a square grid of numbers,  $C_q^i$ .

Note how once again the raw tensor product saw its rank fall by two, from four to two. Also note that the combination of tensor product between two rank-2 tensors, followed by a contraction, to get a new rank-2 tensor, is arithmetically equivalent to matrix multiplication. We can even (although this is rarely applicable) relax the rule that all the indices must be of the same dimension, and only require the indices that we contract to be the same dimension (as of course they must be, otherwise how would they pair up?)

So we've found a generalisation of the dot product and matrix multiplication that extends to tensors of any rank.

Note that in the definition of matrix multiplication, we combine the tensor product and reduction into a single operation, which saves some effort, but it also disguises something: it appears we never have to choose which indices to eliminate in the contraction. Matrix multiplication has a built-in decision to eliminate two specific indices.

This comes from the fact that the matrix indices are classified as either rows (superscript) or columns (subscript), and one matrix is on the left and the other on the right. So multiplying two square matrices  $A$  and  $B$ , to obtain  $C$  we use the same index for the subscript on the left and the superscript on the right:

$$C_j^i = A_n^i B_j^n$$

To spell this out:

$$\begin{bmatrix} C_1^1 & C_2^1 \\ C_1^2 & C_2^2 \end{bmatrix} = \begin{bmatrix} A_n^1 B_1^n & A_n^1 B_2^n \\ A_n^2 B_1^n & A_n^2 B_2^n \end{bmatrix} = \begin{bmatrix} A_1^1 B_1^1 + A_2^1 B_1^2 & A_1^1 B_2^1 + A_2^1 B_2^2 \\ A_1^2 B_1^1 + A_2^2 B_1^2 & A_1^2 B_2^1 + A_2^2 B_2^2 \end{bmatrix}$$

If we instead used the same index for the left superscript and the right subscript, we wouldn't get the same answer.

$$A_i^n B_n^j \neq A_n^i B_j^n$$

But if we then reverse the order of the matrices, which does not affect the answer, we restore the "left subscript, right superscript" rule:

$$A_i^n B_n^j = B_n^j A_i^n$$

And this is exactly what we find with matrix multiplication. By interchanging the two input matrices, we effectively change the decision as to which indices to eliminate in the contraction, and that is why matrix multiplication is non-commutative.

## 4.5 Tensors as geometric objects

The point of tensors is to produce the same value from a computation regardless of the coordinate system chosen. This means the tensor is a geometric object: its description in terms of coordinates is not fundamental. It has magnitude and direction (if rank-2 it has two directions, and so on.)

It also means that for a tensor there is a rule governing how its coordinates must change under a change of basis. The whole point of this rule is to ensure that the change of basis does not affect the result.

If we treat a rank  $N$  tensor as a scalar-valued function of  $N$  vectors, some changes of basis will make no difference to the result, but others will. Those transformations to the basis under which the scalar value of a tensor is invariant are commonly known as rotations, although they also include mirroring.

A well known example of a scalar valued function of two vectors is the dot product, which depends on the length of the two vectors and the angle between them. A rotation changes none of these factors. Whereas a scale change will change the number used to measure each vector's length, and so must change the output. It's no different from deciding to work in yards rather than metres.

## 4.6 Tensors as functions

Sometimes a tensor is defined as a scalar valued function of vectors. It might be more accurate to say that any tensor *can be employed* as such, i.e. a function that accepts  $n$  vectors (given by its rank,  $n$ ) and produces a scalar. However, in the same way, supposing its rank is high enough, it can be employed as a function that accepts  $n - 1$  vectors and produces a vector, or accepts  $n - 2$  vectors and produces a matrix, etc.

If  $T$  is a rank-3 tensor with coordinates  $T_{ijk}$ , and if we have three rank-1 tensors (vectors) with coordinates  $A^i$ ,  $B^j$  and  $C^k$  we can evaluate  $T$  by summation notation:

$$T(\mathbf{A}, \mathbf{B}, \mathbf{C}) = T_{ijk} A^i B^j C^k = \sum_i \sum_j \sum_k T_{ijk} A^i B^j C^k$$

This is not purely the tensor product - we've also chosen to perform contraction three times, by repeating each of the three indices.

What happens if we only have two vectors available to us at the moment? We can partially apply the tensor:

$$T(\_, \mathbf{B}, \mathbf{C}) = T_{ijk} B^j C^k = \sum_j \sum_k T_{ijk} B^j C^k = V_i$$

Note that in the component summation, the index  $i$  is not summed over - it's unbound, or free, and so the expression is a way to compute the  $i$ -th component of a vector  $\mathbf{V}$ . So in a sense, we have treated the rank-3 tensor as a vector-valued function of two vectors. Or if you prefer, a function of two vectors that produces a function of one vector.

But we can "finish the job" whenever we obtain  $\mathbf{A}$ :

$$\mathbf{V}(\mathbf{A}) = V_i A^i = \sum_i V_i A^i$$

And we have no free indices, so the result is a scalar. This freedom to apply  $T$  to  $\mathbf{B}$  and  $\mathbf{C}$  first, and then apply the result of that to  $\mathbf{A}$ , shuffling the order of operations, is part of the essence of tensors. Ultimately all we are doing is multiplying sets of numbers, and then summing them up, so the order in which we do these things is up to us; it makes no difference to the result, *as long as we are consistent* in matching subscript indices to superscript indices.

## 4.7 Metric tensor

To define the distance between two points in space, we can think of a vector reaching from one point to the other. So we just want to compute the length of that delta-vector,  $\mathbf{D}$  from its coordinates.

In Euclidean space with an orthonormal basis, we use Pythagoras's theorem, which just means that we take the dot product of the vector with itself to get the squared length.

But the dot product is a contraction of rank-2 tensor resulting from the tensor product of the vector with itself. If we don't do the contraction, we get the square matrix  $\mathbf{S}$ :

$$S_{ij} = D_i D_j$$

The diagonal of  $S$  is just the squares of the coordinates, the ingredients needed for Pythagoras. The other elements are all possible combinations of the coordinates. We can use a matrix  $g_{ij}$  to pick out the ingredients we want to include in our sum:

$$s = g_{ij} S^{ij}$$

So  $g_{ij}$  is an example of a tensor being used as a function, specifically a scalar-valued function of two vectors. If we give it two different vectors it gives us the inner product of them, and if we give it the same vector twice, it gives us the square of the magnitude of that vector.

In Euclidean space,  $g_{ij}$  is simply the Kronecker delta, so that only the diagonal elements are included in the sum. In curved space it has other values.

Note that there is much redundancy in such a matrix because  $D_1 D_2$  is the same as  $D_2 D_1$ . For example, in a 4-dimensional space there are 16 matrix elements but only 10 are needed (the 4 of the diagonal and 6 from either side of the diagonal). But sometimes we might be dealing with matrix elements that are not commutative under multiplication, in which case every element of the metric might make a different contribution.

## Chapter 5

# Geometric Algebra

A general way of defining the product of two vectors, as the sum of two other kinds of product:

$$\vec{u}\vec{v} = \vec{u} \cdot \vec{v} + \vec{u} \wedge \vec{v}$$

The first is the familiar dot product that produces a scalar. The second is the *external product* and its result is something called a *bivector*. The question naturally arises, how can we sum a scalar and an exotic new object? But we can brush over this question much as we do with complex numbers, in which we sum a real and imaginary component without requiring them to reduce to a single term.

Geometrically a vector is defined by three things:

- its length (or *magnitude*, a scalar)
- the line it sits in
- in which of the two available directions on the line it is pointing.

A bivector is a flat bounded surface only defined by three things:

- its area (or *magnitude*, a scalar)
- the plane it sits in (sometimes called *attitude* or *orientation*)
- in which of the two available directions it faces (also sometimes called *orientation*, perhaps better described as *direction*), and also conceivable as a direction of rotation.

It follows that the exact shape of the boundary around the area of a bivector is irrelevant. To form a bivector from vectors  $\vec{u}$  and  $\vec{v}$ , where  $\vec{u}$  points to the right and  $\vec{v}$  slants up and to the right, make a parallelogram from them, with sides:  $\vec{u}$ ,

$\vec{v}$ ,  $-\vec{u}$ ,  $-\vec{v}$ . The cycle of vectors follows an anti-clockwise route, which characterises the direction of the bivector. Equivalently, by rotating  $\vec{u}$  anti-clockwise we can align it with  $\vec{v}$ .

By the right-hand rule, if a bivector is anti-clockwise then it is pointing toward you, whereas if it is clockwise then it is pointing away from you. It has a "front" and a "back".

We can picture a circle (or any other shape) with the same area embedded in the same plane and imagine it rotating anti-clockwise, and this would be a way to picture the very same bivector.

A bivector with area zero is the zero bivector (whereupon the attitude and direction of rotation become meaningless.)

Another circle in the same plane with the same area, but rotating *clockwise*, would be the negation of the first bivector. We can also construct this by tracing the parallelogram:  $\vec{v}$ ,  $\vec{u}$ ,  $-\vec{v}$ ,  $-\vec{u}$ , i.e. having  $\vec{u}$  and  $\vec{v}$  switch places. Following the direction of the vectors we cycle clockwise.

Combining two vectors in this way to form a parallelogram is the *external product*, and because if we exchange the vectors the product is negated, we say it is *anticommutative*:

$$\vec{u} \wedge \vec{v} = -\vec{v} \wedge \vec{u}$$

If  $\vec{u}$  and  $\vec{v}$  are colinear then the parallelogram would be of area zero, so the result is the zero bivector (so any vector squared is zero).

Returning to the full geometric product:

$$\vec{u}\vec{v} = \vec{u} \cdot \vec{v} + \vec{u} \wedge \vec{v}$$

The product of a vector with itself is:

$$\vec{u}^2 = \vec{u}\vec{u} = \vec{u} \cdot \vec{u} + \vec{u} \wedge \vec{u}$$

The dot product is just the scalar  $|\vec{u}|^2$ , and we just noted that the external product of any vector with itself is zero, so:

$$\vec{u}^2 = |\vec{u}|^2$$

It follows that in an orthonormal basis, the geometric product of any basis vector with itself is 1. The geometric product of two different basis vectors is a pure bivector with no scalar part, and (by anticommutativity) we can flip the sign by switching the two vectors.

Furthermore, because division is meaningful on scalars we can say for any vector  $\vec{u}$ :

$$\frac{\vec{u}^2}{\vec{u}^2} = 1$$

And so we can give a meaning to *the inverse of a vector*:

$$\frac{\vec{u}}{\vec{u}^2} = \vec{u}^{-1}$$

Multiplying by such an inverse is equivalent to division, but as always the order of the operands is important.

Due to the exterior product being anticommutative, if we switch vectors around the sign changes on the external product part:

$$\vec{v}\vec{u} = \vec{u} \cdot \vec{v} - \vec{u} \wedge \vec{v}$$

First let's add the two orderings:

$$\vec{v}\vec{u} + \vec{v}\vec{u} = \vec{u} \cdot \vec{v} + \vec{u} \wedge \vec{v} + \vec{u} \cdot \vec{v} - \vec{u} \wedge \vec{v}$$

So the external parts cancel leaving:

$$\vec{v}\vec{u} + \vec{v}\vec{u} = 2\vec{u} \cdot \vec{v}$$

$$\frac{\vec{v}\vec{u} + \vec{v}\vec{u}}{2} = \vec{u} \cdot \vec{v}$$

And so we have a way of computing the scalar product in terms of the geometric product.

Then we repeat this exercise but subtracting:

$$\vec{v}\vec{u} - \vec{v}\vec{u} = \vec{u} \cdot \vec{v} + \vec{u} \wedge \vec{v} - \vec{u} \cdot \vec{v} + \vec{u} \wedge \vec{v}$$

This time the scalar parts cancel leaving:

$$\vec{v}\vec{u} - \vec{v}\vec{u} = 2\vec{u} \wedge \vec{v}$$

$$\frac{\vec{v}\vec{u} - \vec{v}\vec{u}}{2} = \vec{u} \wedge \vec{v}$$



And similarly we have a way of computing the external product in terms of the geometric product.

Alternatively we can write  $\vec{u}$  and  $\vec{v}$  in terms of an orthonormal vector basis  $e_i$  with scalar coordinates  $u_i$  and  $v_i$ , and write down the product  $\vec{u}\vec{v}$ :

$$\vec{u}\vec{v} = \sum_i u_i e_i \sum_j v_j e_j = \sum_{ij} u_i v_j e_i e_j$$

We can arrange this in a square matrix of terms, rows  $i$  and columns  $j$ :

$$M_{ij} = u_i v_j e_i e_j$$

The members on the diagonal (where  $i = j$ ) are just  $u_i u_i e_i^2$  and we know that the geometric square of a unit vector is 1, so the sum of the diagonal terms on their own (known as the *trace* of  $M$ ) is just the dot product.

The other terms of the sum include diagonally opposite pairs such as:

$$v_1 u_2 \vec{e}_1 \vec{e}_2 + v_2 u_1 \vec{e}_2 \vec{e}_1$$

We know that  $\vec{e}_1 \vec{e}_2 = -\vec{e}_2 \vec{e}_1$ , so the above can be written as:

$$v_1 u_2 \vec{e}_1 \vec{e}_2 - v_2 u_1 \vec{e}_1 \vec{e}_2 = (v_1 u_2 - v_2 u_1) \vec{e}_1 \vec{e}_2$$

In three dimensions there are three such pairs:

$$(u_1 v_2 - u_2 v_1) \vec{e}_1 \vec{e}_2 + (u_2 v_3 - u_3 v_2) \vec{e}_2 \vec{e}_3 + (u_1 v_3 - u_3 v_1) \vec{e}_1 \vec{e}_3$$

Weirdly, this is the formula for the cross product  $\vec{u} \times \vec{v}$  but with a slight difference:

$$\vec{u} \times \vec{v} = (u_1 v_2 - u_2 v_1) \vec{e}_3 + (u_2 v_3 - u_3 v_2) \vec{e}_1 + (u_1 v_3 - u_3 v_1) \vec{e}_2$$

In fact if we multiply the cross product by  $\vec{e}_1 \vec{e}_2 \vec{e}_3$  we recover the external product, because for example in  $\vec{e}_1 \vec{e}_2 \vec{e}_3 \vec{e}_3$  the repeated  $\vec{e}_3$  factors equal 1, so in each term we replace the basis vector with the (bivector) product of the other two basis vectors.

In each term we've written a bivector in place of a vector perpendicular to it. Physicists often represent a rotation with a vector perpendicular to the plane of rotation, using the right-hand rule to relate the direction of rotation to the direction of the vector (a vector pointing away from you represents clockwise rotation from your perspective). It's known as a *pseudovector* because in physics

the term vector is restricted to describing objects that transform in the expected way under a change of basis, and such pseudovectors do not.

But if we avoid literal pseudovectors and stick with bivectors then this problem is avoided. A bivector is a rank 2 tensor and as such it transforms correctly. In physics all uses of the cross product would be better represented as producing a bivector.

Furthermore, if you think of a rank N tensor as a function that accepts a vector and produces a rank N-1 tensor, how does that relate to multivectors?

A bivector  $A$  multiplied by a vector  $\vec{w}$  is like the product of two vectors  $\vec{u}\vec{v}$  multiplied by a vector:

$$A\vec{w} = \vec{u}\vec{v}\vec{w}$$

Any vector  $\vec{u}$  can be written as a weighted sum of the orthogonal basis vectors, the weightings  $u_i$  being the components of the vector:

$$\vec{u} = \sum_i u_i e_i$$

$$A\vec{w} = \sum_{ijk} u_i v_j w_k e_i e_j e_k$$

This isn't a square matrix, but it is a cube-shaped object. It's a trivector, which as we will see is not a scalar but in  $\mathbb{R}^3$  has only choice of "orientation" (just like a bivector in  $\mathbb{R}^2$  only has one choice of plane to lie in) so the only properties that we can use to distinguish two trivectors are the magnitude and sign, so in  $\mathbb{R}^3$  a trivector is a pseudoscalar.

As the geometric product is the sum of the dot product (which we found on the diagonal of our matrix) and the external product (which we found in all the other members), we can think of the geometric product as the sum of two matrices:

$$\vec{u}\vec{v} = \begin{bmatrix} u_1 v_1 & 0 & 0 \\ 0 & u_2 v_2 & 0 \\ 0 & 0 & u_3 v_3 \end{bmatrix} + \begin{bmatrix} 0 & u_1 v_2 & u_1 v_3 \\ u_2 v_1 & 0 & u_2 v_3 \\ u_3 v_1 & u_3 v_2 & 0 \end{bmatrix}$$

Just as a bivector is an area with an orientation, a *trivector* is a volume with an orientation.

But note that this orientation is not like the ability of some specifically-shaped solid to be rotated in  $\mathbb{R}^3$ .

- A trivector has no shape, so for simplicity visualise it as a sphere, and note that the normal sense of rotation will have no effect on it, and cannot be a distinguishing property. So that's not what we mean by orientation in this context.
- Consider how a bivector in  $\mathbb{R}^2$  only has one choice of plane to lie in, whereas in  $\mathbb{R}^3$  it can choose from an infinity of planes akin to  $\mathbb{R}^2$  that are embedded in  $\mathbb{R}^3$ . The bivector will have no extent orthogonal to its chosen plane, but only exists as an area within that plane.
- Analogously a trivector in  $\mathbb{R}^3$  has no choice about what space its volume exists in, but in  $\mathbb{R}^4$  there is an infinity of possible hyperplanes (three dimensional "slices" of  $\mathbb{R}^4$ ) to choose from. A trivector exists as a volume in only one such hyperplane, and has no extent in the remaining orthogonal direction.
- For a trivector orientation only becomes a distinguishing property in  $\mathbb{R}^4$  or higher.

A trivector can be constructed as the product of three vectors, producing a paralleliped, a six-faced figure. Each face is a bivector (just as each side of a bivector is a vector). Higher-dimensioned forms follow similarly. All of these are known as *k-vectors*.

A linear combination of orthonormal basis k-vectors is called a multivector. So in two dimensions where we have basis vectors  $\vec{e}_1, \vec{e}_2$ , the available k-vectors are:

- scalars (multiples of 1)
- multiples of  $\vec{e}_1$
- multiples of  $\vec{e}_2$
- multiples of the bivector  $\vec{e}_1\vec{e}_2$

So in two dimensions all multivectors  $x$  are described by 4 components,  $x_i$ :

$$x_1 + x_2\vec{e}_1 + x_3\vec{e}_2 + x_4\vec{e}_1\vec{e}_2$$

In three dimensions we have:

- scalars (multiples of 1)
- multiples of  $\vec{e}_1$
- multiples of  $\vec{e}_2$
- multiples of  $\vec{e}_3$
- multiples of the bivector  $\vec{e}_1\vec{e}_2$
- multiples of the bivector  $\vec{e}_2\vec{e}_3$

- multiples of the bivector  $\vec{e}_1 \vec{e}_3$
- multiples of the trivector  $\vec{e}_1 \vec{e}_2 \vec{e}_3$

and therefore 8 components in a multivector:

$$x_1 + x_2 \vec{e}_1 + x_3 \vec{e}_2 + x_4 \vec{e}_3 + x_5 \vec{e}_1 \vec{e}_2 + x_6 \vec{e}_2 \vec{e}_3 + x_7 \vec{e}_1 \vec{e}_3 + x_8 \vec{e}_1 \vec{e}_2 \vec{e}_3$$

Note how in each case there is one term made of all the vectors:

- $x_4 \vec{e}_1 \vec{e}_2$  (2 dimensions)
- $x_8 \vec{e}_1 \vec{e}_2 \vec{e}_3$  (3 dimensions)

so there is only one component for it. This makes it similar to a scalar and it's known as a pseudoscalar.

Also in  $N$  dimensions there is a set of terms made of  $N - 1$  vectors, i.e. using all basis vectors except one, and there are  $N$  such components, just like a vector:

- $x_2 \vec{e}_1 + x_3 \vec{e}_2$  (2 dimensions)
- $x_5 \vec{e}_1 \vec{e}_2 + x_6 \vec{e}_2 \vec{e}_3 + x_7 \vec{e}_1 \vec{e}_3$  (3 dimensions)

so these together form a pseudovector.

These terms that are the products of vectors are called *blades*. The number of vectors that go into making blade is call the *grade*. A 0-blade is a scalar, and in  $N$ -dimensions an  $N$ -grade is a pseudoscalar, whereas  $(N - 1)$ -grade is a pseudovector.

Even when constrained to two dimensions, with orthonormal basis  $\vec{e}_1, \vec{e}_2$  bivectors have their uses. The bivector  $\vec{e}_1 \vec{e}_2$ , which can be pictured as a square with a cycle of vectors  $\vec{e}_1, \vec{e}_2, -\vec{e}_1, -\vec{e}_2$  around its edge, can be multiplied by itself via the geometric product:

$$(\vec{e}_1 \vec{e}_2)^2 = \vec{e}_1 \vec{e}_2 \vec{e}_1 \vec{e}_2 = -\vec{e}_2 \vec{e}_1 \vec{e}_1 \vec{e}_2 = -\vec{e}_2 \vec{e}_2 = -1$$

So the bivector  $\vec{e}_1 \vec{e}_2$  gives the value  $-1$  when squared, which means that in geometric algebra, we have a way of defining  $i$  for any given plane: the product of two orthogonal unit vectors in that plane.

As usual, it represents a  $\pi/2$  or 90-degree rotation, but with one difference due to the anticommutative nature of the geometric product:  $\vec{a}i$  equals  $i$  (clockwise rotated), whereas  $i\vec{a}$  equals  $-i$  (anti-clockwise).

As a bivector is only characterised by its magnitude (area), the plane it lies in (in this case we're only considering two dimensions so there's no freedom here), and the direction of rotation (clockwise or anti-clockwise), this latter being equivalent to a change of sign, all bivectors in the plane can be written as

scalar-multiples of the unit bivector  $i$ . So in fact in two dimensions any multivector is the sum of a scalar and a scalar-multiple of  $i$ . This means that a complex number can be viewed as a multi-vector in  $\mathbb{R}^2$ :

$$a + bi$$

Furthermore a change to the sign of the "imaginary part" is the same as the complex conjugate, and this is what happens when a geometric product has its operands switched.

Note that we normally think of  $i$  as a scalar, and therefore it is no coincidence that we've discovered that it is actually a pseudoscalar, a blade (in  $N$  dimensions, an  $N$ -vector that is the product of  $N$  1-vectors).

Much of what has been said here about 2 dimensions holds true in 3. The highest grade is the trivector  $\vec{e}_1\vec{e}_2\vec{e}_3$  and this again serves as the pseudoscalar and is labelled  $i$ , and  $i^2 = 1$  as before.

But unlike 2 dimensions, in 3 dimensions  $i$  commutes with all multivectors:

$$iA = Ai$$

We can also think of the wedge product as a way to characterise the non-commutativity of two vectors under the tensor products.

$$\vec{u} \wedge \vec{v} = \vec{u} \otimes \vec{v} - \vec{v} \otimes \vec{u}$$

So the matrix element at  $i, j$  is given by:

$$(\vec{u} \wedge \vec{v})_{ij} = u_i v_j - u_j v_i$$

## Chapter 6

# Potential

A force field is a vector-valued function of space, i.e. at each point in space we imagine there is a vector giving the strength and direction of the force that would be felt at that point.

The force fields we observe in nature have an interesting property: it is always possible to replace the force field with a scalar-valued function of space, i.e. at each point in space there is merely an ordinary number, not a vector. We can then take the vector gradient  $\nabla$  of this scalar field and we recover the force field.

By analogy, picture a hilly landscape. The height  $H$  above sea level is the scalar field value, so the landscape is fully described by the scalar field  $H(x, y)$ . From this we can derive  $\nabla H$ , a two-dimensional vector field (picture it as an arrow that never points up or down, always parallel to the horizon). As we travel around we sometimes face steep slopes, where  $\nabla H$  points in the steepest direction, or stationary points such as hilltops or valley basins where  $\nabla H$  is the zero vector (to distinguish between peaks and valleys, we'd need to take the second derivative,  $\nabla^2 H$ ).

If we wander on some pathway through this landscape and return back to where we started, our height will be the same as it was when we started (assuming the landscape hasn't changed shape). This is true regardless of the path we take, as the height is a fact about the start/end point of the path. This is so obvious as to seem hardly worth stating.

And yet if we only had some vector field, and wondered if the path integral of any closed loop through that field was always zero, how would we know? Some paths might go mainly through regions with vectors all pointing in one direction, and so not sum to zero. Not all vector fields have this self-balancing property.

Those that do are known as conservative fields, and these are fields which can

be reduced to a scalar field from which the vectors can be recovered by applying  $\nabla$ , and these are all the force fields we encounter in nature.

When we describe a force field by a scalar field, we call that field a *potential*. It has units of energy. As a particle moves through a potential, it experiences a potential difference between two points. If this difference is negative, i.e. the potential energy drops between the two points, the particle gains kinetic energy (speeds up). This is exactly like a ball rolling down a slope; the potential energy is exactly equivalent to the height of the landscape.

If the potential does not vary, the gradient is zero. This is true regardless of the potential's constant value, which is like a constant of integration, i.e. a global increase in potential is physically meaningless.

## Chapter 7

# Expectation Value

This unfortunate statistical term is used everywhere; unfortunate because it describes a value that we do not necessarily expect to ever measure, and even more unfortunate that it is often garbled into “the expected value”, which may be entirely untrue. It is the expected *mean* of a set of repeated measurement values.

For a set of discrete values taken by some integer variable  $n$ , the values may be 2, 3, 3, 3, 4, 4, 5, which sums to 24, and there are 7 values, so the mean value is 3.42857... which is not an integer so clearly cannot be an expected value.

Looking at the list of values, we can tabulate them by giving the observed (“frequentist”) probability  $P$  of each value (number of times it occurs divided by the size of the set of values):

$n$	$P_n$
2	1/7
3	3/7
4	2/7
5	1/7

$P_n$  is zero for all  $n$  except the above exceptions, where it is between zero and 1, and of course all values of  $P_n$  add up to 1 because we fixed them to do that when we divided them all by 7.  $P_n$  is literally “what fraction of the 7 values is contributed by  $n$ ”.

Therefore by computing the weighted sum:

$$\langle n \rangle = \sum_n n P_n$$

we recover the mean value  $\langle n \rangle$ . The point here is that, inside a sum at least, it



makes sense to multiply a value by the probability of obtaining that value.

In the continuous case, the probability density function  $\rho(x)$  does not give us the probability of  $x$ , a meaningless concept for a continuous variable (any specific value is infinitesimally unlikely), but it can be integrated over some region to get the probability of the value appearing in that region.

The integral over all values of  $x$ :

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x) dx$$

is the continuous equivalent of (1) and gives the mean value of a large set of measurements of  $x$ . If we think of all the values of  $x$  as a cloud of matter that is more or less densely concentrated here or there,  $\langle x \rangle$  is like its centre of mass.

But  $\rho(x)$  may be symmetrical around the origin and vanish at the origin, e.g. two peaks on either side, making  $\langle x \rangle = 0$  despite  $x$  never taking the value 0; so if we are required to call it "the expectation value", we must always remember that it may be a value that never occurs.

## Chapter 8

# Fourier Transform

Given a real-valued function  $f(x)$ , and supposing it is periodic, e.g. it describes the sound of a bell ringing, you might ask what frequencies appear in the sound. In fact your ear-brain system is an adaptation for answering that very question, and if you listen carefully you can often discern several different notes within the sound of a bell.

What we're really asking is how "loud" the signal is at each frequency. We can detect this for a given frequency  $\nu$  by multiplying the function by  $e^{-i2\pi\nu x}$ , in which:

- the minus sign is purely a convention (and not a universal one)
- $i$  is the magic ingredient that makes it go round and round
- $2\pi$  converts to radians
- $\nu$  is the frequency
- $x$  is the parameter to the function

So if  $\nu$  is 1, the complex value performs a whole rotation as  $x$  goes from 0 to 1, and again from 1 to 2, etc.

By itself this factor is a unit complex number, i.e. of "length" 1, but by multiplying it by the function we adjust its length so it oscillates "in and out" as it rotates, exactly like our signal:

$$f(x)e^{-i2\pi\nu x}$$

If the oscillations of  $f$  don't coincide with the frequency  $\nu$ , the above expression will, averaged over all values of  $x$ , be about zero, there being no particular reason for the complex value to be biased in any direction. That is:

$$\int_{-\infty}^{\infty} f(x)e^{-i2\pi\nu x} dx \approx 0$$

But if the oscillations do coincide, then there will be a bias; each time the oscillation of  $f(x)$  reaches a maximum it will be on the same side of the circle traced by  $e^{-i2\pi\nu x}$ .

(A minor subtlety is that whenever  $f(x)$  is at a negative minimum,  $e^{-i2\pi\nu x}$  will be on the other side of the circle; however, multiplying it by the negative value of  $f(x)$  will flip it round by 180 degrees, so both positive peaks and negative troughs will both contribute to the same biased direction.)

So we can define a complex-valued function of frequency:

$$\hat{f}(\nu) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi\nu x} dx \quad (8.1)$$

and this will be about zero for frequencies that don't appear in the function, and non-zero for frequencies that do appear. These values are *complex* amplitudes; they tell us how loud the signal is at that frequency, but also their phase tells us how the signal is offset at that frequency.

As a shorthand we can write it as a fancy  $\mathcal{F}$ :

$$\hat{g} = \mathcal{F}g$$

We can do the opposite transformation:

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\nu)e^{i2\pi\nu x} d\nu \quad (8.2)$$

Shorthand:

$$g = \mathcal{F}^{-1}\hat{g}$$

This pretty much literally says that you can make any function by adding together an infinite collection of oscillations at every possible frequency. You just need a (complex) function  $\hat{f}(\nu)$  that tells you how "loud" each frequency needs to be.

## 8.1 Negative Frequencies

By the way, note how when we do the integral over  $\hat{f}$  in the inverse transform, we include negative values. What on earth is a negative frequency?! It's not that weird, really. It just makes the complex factor rotate the other way. This underscores the fact that the minus sign is just a convention. The integrals cover both "directions".

There's a special relationship between the positive and negative sides of the frequency spectrum. According to equation (8.1), if you want the amplitude for frequency  $-\nu$ , it must be:

$$\hat{f}(-\nu) = \int f(x)e^{i2\pi\nu x}dx$$

Which means  $\hat{f}(-\nu)$  is the complex conjugate of  $\hat{f}(\nu)$ .

$$\hat{f}(-\nu) = [\hat{f}(\nu)]^*$$

Therefore having done the hard work of computing one side, it is very easy to get the other side - it contains no different information.

Also, note that as we're integrating over all  $x$  from  $-\infty$  to  $\infty$ , we can negate  $x$  through the integral without changing the result. So this produces the exact same frequency amplitudes as equation (8.1):

$$\hat{f}(\nu) = \int f(-x)e^{i2\pi\nu x}dx$$

Suppose  $f$  happens to be an even function:

$$f(-x) = f(x)$$

Then we can switch freely:

$$\hat{f}(\nu) = \int f(x)e^{i2\pi\nu x}dx$$

If we mirror the frequency:

$$\hat{f}(-\nu) = \int f(x)e^{-i2\pi\nu x}dx$$

But we've arrived back at equation (8.1), meaning it must be perfectly symmetrical around  $\nu = 0$  when applied to an even function. This means it must also be real at all frequencies - how else could all this be true?

$$\hat{f}(-\nu) = \hat{f}(\nu) = [\hat{f}(\nu)]^*$$

Now suppose  $f$  is odd:

$$f(-x) = -f(x)$$

By a similar argument, when we substitute:

$$\hat{f}(\nu) = - \int f(x) e^{i2\pi\nu x} dx$$

And mirror:

$$\hat{f}(-\nu) = - \int f(x) e^{-i2\pi\nu x} dx = -\hat{f}(\nu)$$

If taking the complex conjugate is the same as negating, we must be talking about a purely imaginary number. So the transform of an odd function is imaginary and odd.

## 8.2 Spikes

What happens if we take the Fourier transform of a pure *sin* wave? Only a single frequency is present, so it must have the amplitude 1 while all other frequencies are amplitude 0. This is not a smooth curve, but rather a single spike. If we integrate it over all frequencies we get 1, contributed entirely by the spike at one place. This is known as the Dirac delta,  $\delta$ , and is often referred to as a function, or a "function" with scare-quotes. It has a number of strange properties if regarded as a function, so it's simpler to think of it as only ever appearing as a factor inside an integral.

We can move the spike from zero to the location of our choice,  $\alpha$ , with an expression like  $\delta(x - \alpha)$ . It's like the real number equivalent of the Kronecker delta, though we write that slightly differently. You can think of the Kronecker  $\delta_{nm}$  (§2.4) as meaning the same thing as Dirac  $\delta(n - m)$ : if  $n = m$ , the result is 1, otherwise 0.

So if we have a set of complex amplitudes  $A_n$  at frequencies separated by  $\alpha$ , we can put a spike at each:

$$\hat{f}(\nu) = \sum_n A_n \delta(\nu - n\alpha)$$

The result is that the spectrum  $\hat{f}(\nu)$  has spikes of the required amplitude at equally spaced frequencies. So in this way,  $\delta(\nu - n\alpha)$  is like a logical test for whether frequency  $\nu$  matches  $n\alpha$ , and if so,  $\nu$  has amplitude  $A_n$ .

A strange way to think about any function is to regard it as the sum of an infinite set of spikes, one for each possible value of the function's parameter. So for a function of a real parameter, it is an uncountable, continuous set of spikes. What would be a way to describe the height of a given spike? The function itself, of course. A function  $f(y)$  returns you the height of the spike for parameter  $y$ . We can build the function from all the spikes via an integral:

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

To get the value of  $f(x)$  for one value of  $x$ , we're apparently considering every possible value  $f(y)$ , but we discard all of them except where  $y = x$ , because that is the only case where the  $\delta$  is 1, so it picks out the only value we want. It's completely redundant though! We're defining the function in terms of itself. Or rather, we're defining the Dirac  $\delta$ ; the above could only be correct if it has the particular behaviour we've described.

### 8.3 The Gaussian

An infinitesimally narrow spike in the frequency spectrum represents the single frequency present in a pure wave that goes on forever. And a pure wave in the frequency spectrum represent the infinite set of frequencies that must be summed to get an infinitesimally narrow spike. Each is the Fourier transform of the other. They are the two extremes of:

- being localised in position but spread out in frequency - being spread out in position but localised in frequency

Between these two there is a middle ground, a shape that is its own Fourier transform. The best known example is the Gaussian, of the form:

$$g(x) = Ae^{Bx^2}$$

Where  $A$  and  $B$  are constants. There are several ways of concluding that its Fourier transform is:

$$\hat{g}(\nu) = A\sqrt{\pi/B}e^{-\frac{\pi^2}{B}\nu^2}$$

This is evidently of the same form. Aside from being a function of frequency  $\nu$  instead of position  $x$ , the constant  $A$  has become  $A\sqrt{\pi/B}$ , and  $B$  has become  $-\frac{\pi^2}{B}$ , and these are just different constants.

## Chapter 9

# Quantum Mechanics

### 9.1 State Vectors and Dirac Notation

In quantum mechanics everything knowable about the state of some system is described in a vector, known as the state vector. The vector is from a vector space defined over the field of complex numbers, so it is important to use the correct definition of the inner product (§3.12) where we take the conjugate of one of the vectors, to ensure that the inner product of a vector with itself is a non-negative a real number.

The inner product in this context is written like this:

$$\langle a|b\rangle$$

If the vectors  $\vec{a}$  and  $\vec{b}$  are represented by column matrices  $a$  and  $b$  (to spare ourselves, for the moment, from things we can't imagine, let's pretend we're discussing a finite-dimensional vector space), the above is equivalent to conjugate-transpose of  $a$ , written as  $a^\dagger$  ("a-dagger"), matrix-multiplied by  $b$ :

$$a^\dagger b$$

We can split this inner product notation into separate pieces, so we can write  $\langle a|$  to mean the vector whose matrix representation in some basis is a single row containing the complex conjugates of the elements in the single column of the matrix representing  $|a\rangle$  in the corresponding dual basis.

Or more simply,  $\langle a|$  is the covector of  $|a\rangle$ . The convention is therefore to think of  $\langle a|$  as a function that extracts the coordinate of a basis vector  $|a\rangle$  from its argument, which will be some vector  $|b\rangle$ , as in the expression  $\langle a|b\rangle$ . And in concrete matrix terms we can picture  $\langle a|$  as a 1-row matrix (a row vector) that



is the dual of the 1-column matrix (column vector)  $|a\rangle$ , and their corresponding coordinates are mutually complex conjugates.

And with this in mind, it follows that we can write them the other way round from the inner product:

$$|b\rangle\langle a|$$

which must therefore define a matrix: the product of a column vector on the left and a row vector on the right. This is the *outer* product. A matrix can act as a vector-valued function of vectors: apply it to a vector to transform that vector to another vector. So:

$$|b\rangle\langle a|c\rangle$$

See how the notation nicely suggests we bracket the  $\langle a|c\rangle$  first as an inner product and thus a mere number. So we immediately know that the result will be the vector  $|b\rangle$  scaled by a number, i.e. it will be co-linear with  $|b\rangle$ . We've measured  $|c\rangle$  against  $|a\rangle$  and used that to scale  $|b\rangle$ .

Given an orthonormal basis  $|b_n\rangle$ , we can picture it as a set of  $n$  column vectors, and expressed in their own basis they would be the standard basis. The outer product:

$$|b_n\rangle\langle b_n|$$

will produce a matrix with a single 1 in one place of the diagonal. So if we sum over all  $n$ , we get the identity matrix, a matrix that makes no difference to whatever vector it applies to. Spelling this out, if our vector space has just two basis vectors:

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

and

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

Then the outer product of  $|0\rangle$  with itself is just:

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

and likewise of  $|1\rangle$  with itself:

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

And as predicted, summing those matrices gives the identity matrix:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Even if the  $|b_n\rangle$  were expressed in some other basis, the above summation would still be the identity matrix. Now for any vector  $|c\rangle$  we can construct for each  $n$ :

$$|b_n\rangle\langle b_n|c\rangle$$

The  $|b_n\rangle\langle b_n|$  operator is called a projection operator, because it projects its argument onto the subspace spanned by  $|b_n\rangle$ , resulting in a component vector of the argument in the direction of  $|b_n\rangle$ . Clearly if we act with the same projection operator again on that result, nothing will change, because it's already projected. This is a way of defining a projection operator: it's idempotent.

And the sum of all those resulting vectors for all  $n$  will just be  $|c\rangle$ , of course, because we've done the equivalent of acting with the identity operator.

## 9.2 Hilbert Spaces

The vector spaces used to represent physical states are examples of Hilbert spaces, which for our purposes means that:

- they have an inner product that we can use to get a non-negative real number for the modulus of a vector:  $\sqrt{\langle a|a\rangle}$ , and
- they may be infinite dimensional.

The latter possibility includes infinities that are continuous (uncountable). Such vectors cannot be represented by a column of discrete values, not even an infinitely long column. Instead we have to specify a complex-valued function over a continuous (real) variable. Such functions can be added and scaled, as is required of a vector (§1) and so they qualify as elements of a vector space (§3.2) and we therefore have no choice but to admit that they are vectors.

The real value is analogous to the integer index that labels the rows in a column vector; instead of fetching the  $i$ th component by its position in the column, we evaluate the function with some real value  $x$ .

Similarly, whereas the inner product over discrete components is:

$$\langle a|b\rangle = \sum_i x_i^* y_i$$

the inner product over functions  $f$  and  $g$  of a real variable  $x$  is:

$$\langle f|g\rangle = \int_{-\infty}^{+\infty} f(x)^* g(x) dx$$

This is also called the overlap integral, because it measures the extent to which the two functions overlap, but it is most definitely also the inner product between two vectors. Thus we can in some sense find the square of the "length" of a function:  $\langle f|f\rangle$ . This sounds like gibberish, but it is an unavoidable consequence of the definition of a vector space, which is abstract enough to admit a space of possible functions.

### 9.3 Physical Interpretation

To interpret the state vector physically, we choose a basis so we can resolve it into components. Our choice of basis has to do with the observable quantity we are presently interested in, such as position, momentum, orientation or energy. If it may take on any real value, the state vector will have to be a function of that value; if it may only take on certain discrete values, it can be a column vector (albeit sometimes one with infinitely many rows) in which each row corresponds to one of those possible discrete values that the observable may exhibit when measured.

The information available from the state vector is, in general, probabilistic. Each component, being a complex number, is related to the probability of the observable quantity taking on the value represented by that component. The squared modulus of the component (its value multiplied by the complex conjugate of its value) is the probability of obtaining that value, or if the state vector is a function  $f(x)$ , then:

$$\int_a^b f(x)^* f(x) dx$$

is the probability that  $x$  will have a value somewhere between  $a$  and  $b$ .

As a probability is a number between 0 and 1, it must be the case that the sum of the squared modulus of all the components (or the above integral from  $-\infty$  to  $+\infty$ ) must be 1. This is the same as saying that  $\langle S|S\rangle = 1$  for any physically realistic state vector. Or to put it another way, the magnitude of a state vector is not significant, only the direction (i.e. the relative values of the components in some basis). We will always fix the magnitude to be 1.

Unsurprisingly, if one of the components is 1 and all the others are zero, the vector represents certainty that the observable has the value represented by that component. But this also means that the state vector is equal to one of the basis vectors. Thus the basis vectors for an observable represent exact values that the observable may exhibit when measured.

Further, a measurement of the observable (or more precisely, any interaction producing subsequent behaviour that could be used to infer the value of the observable) causes the state vector to change to the basis vector of that observable corresponding to the measured value. This change is (at least in this theory) assumed to be instantaneous and to have no mechanism that we can deduce anything further about.

Thus after measuring an observable, subsequent measurements of the same observable will with certainty produce the same result.

(This is not quite true in the continuous cases when the state vector is actually a function of a real variable. We don't expect to ever find such a system precisely aligned with a single base state, but instead to have at least some small spread of probabilities.)

## 9.4 Switching Basis

Having constructed a column representation of a state vector in one basis, relating to one observable, we can switch to another. The operation for doing this will depend on both the "before" and "after" bases (§3.5). A state vector contains everything knowable about a system, including all we can know about any of its observable quantities. By re-expressing the same state vector as a different set of components in terms of the basis associated with a different observable, we recover the probability distribution for that observable.

As always when using an operator to transform a vector's components we need to be clear on whether we want to get a different vector in the same basis or the same vector in a different basis. In this case, physically we're talking about the latter; a state vector represents something physically real, and we're just changing how we describe it. On the other hand, mathematically all we have is the description, and the choice of basis is not entirely arbitrary because a basis relates to an observable quantity.

## 9.5 Operators Representing Observables

Observables have an associated operator. Note that this is *not* the same as the operator for converting a state vector to a different basis. In QM when we talk about the observable's associated operator, we are talking about something that is not directly of any use for converting between bases, though it will indicate how we could perform such an operation.

An observable operator can be applied to a state vector as a kind of test, but it is much more powerful when we picture it applying to every possible state vector (that is, all unit vectors in the space) to find out how it affects them.

In QM operators associated with observables are Hermitian or self-adjoint, meaning that for an operator  $\hat{O}$ :

$$\langle a | \hat{O} b \rangle = \langle \hat{O} a | b \rangle$$

This has a few useful implications:

- in the discrete finite vector case, operators can be represented as a matrix  $O$ ,  $O^\dagger = O$ , or  $O_{ij} = O_{ji}^*$ , so the main diagonal elements are real,
- regardless of representation, eigenvectors (§3.8) with distinct eigenvalues are orthogonal and complete (they span the space, so you can take a unit vector in each of these orthogonal directions and you have an orthonormal basis) and
- regardless of representation, their eigenvalues are real.

Think of the analogy of a Euclidean real plane vector space, and a symmetric  $2 \times 2$  matrix  $M$  operating on it. The eigenvectors are lines in the plane along which vectors do not change direction, only magnitude, when the operator is applied. Because the matrix is symmetric ( $M_{ij} = M_{ji}$ ) these lines are orthogonal. So it is with an Hermitian operator in a complex space, with only the added complication of needing to be careful about taking the complex conjugate when comparing diagonally opposite elements.

The basis vectors of the observable are just unit vectors that are eigenvectors of the operator. That is, if you apply the observable's operator to every possible state vector, a subset of them will be scaled (by a potentially complex factor) without any change to their alignment. There will be a set of orthogonal unit vectors that pass this "alignment preserving" test, and these form the basis of the observable.

In other words, quantum mechanics is substantially about:

- defining the operator for an observable,
- solving the eigenvalue equation for that operator (that is, finding its eigenvectors and their associated eigenvalues)
- using the eigenvectors as a basis for representing state vectors,
- assuming that when the observable is measured, the state will snap into alignment with one of those eigenvectors,
- interpreting a coordinate in that basis as a complex amplitude whose mod-square is the probability that the state will align itself with that basis vector,

- interpreting the eigenvalue associated with the basis vector as the measured value of the observable (the eigenvalues of Hermitian operators are real numbers, fortunately.)

If a system's state vector matches one of these eigenvectors, then the system is already in an eigenstate and if the observable is measured, the result will with certainty be the eigenvalue associated with that eigenstate.

Otherwise, the state vector will be a linear combination of the eigenstates, and if the observable is measured and found to have a particular value, then the state vector will have instantaneously realigned itself with an eigenvector having that eigenvalue.

It is therefore very clearly the case that an observable's operator should not be mistaken for a means to transform a state vector into the basis of the observable. Consider a state vector that is already aligned with an eigenstate of the operator, but is currently expressed as a linear combination of some other basis, so it has several non-zero coordinates. But in the basis of the observable, its coordinates should all be zero except for the eigenstate's coordinate, which will have some complex value of modulus 1. The observable's operator clearly cannot bring about this transformation: the state vector's coordinates will all be scaled by the same factor (the eigenvalue), by the very definition of eigenvectors.

But if we solve the eigenvalue equation for the operator, we will know the complete basis of the observable, along with the eigenvalue associated with each basis vector, and we can then resolve our state vector against those basis vectors. Then we will have a set of coordinates that serve as probability amplitudes for the associated (measurable) eigenvalues.

In addition, there is a meaningful interpretation for the result of applying the operator for an observable to a given state vector: the inner product of that vector with the original state vector gives the expectation value (§7) of the observable.

While we've discussed all this in terms of more easily pictured finite-dimensional vectors with discrete complex components, all the same concepts translate to complex-valued functions of an integer or real parameter.

## 9.6 The Wave Function

One way to approach QM initially is to consider the position and momentum of an electron. These are continuous variables, so we will be working entirely with state vectors that are represented by functions of real variables, and operators that transform functions.

We model this situation as a continuous complex-valued function of position and time,  $\Psi(x, y, z, t)$ , very often abbreviated to  $\Psi$ . We will sometimes also

consider functions only of space,  $\psi$ . (This upper/lowercase distinction is quite widespread but not universally observed.)

By considering only one spatial dimension we can picture the wave function at one instant as a line, somewhere along which the electron could be found. At each point  $x$  on the line there is an associated complex plane (visualised as normal to the line), with an arrow lying in it, pointing out from the line. This is the complex value of  $\Psi$  at that position  $x$  and time  $t$ .

The complex plane should not be confused with vectors. Any given snapshot of  $\Psi(x, t)$  at some instant  $t$ , given by a function  $\psi(x)$ , is itself an entire vector. The position  $x$  labels a single infinitesimal component of the vector, and every such component is a complex number, which we can therefore visualise as a complex plane with an arrow on it.

So for example we could picture the arrows as making a corkscrew shape, rotating around the line such that the angle depends linearly on  $x$ , but the modulus of the complex value (the length of the arrow) happens to be constant in this example. This is the notional wave function for a free electron (no forces acting it) with a precisely defined momentum and therefore no defined position, something never observed in reality.

More generally, the arrow length will also vary with  $x, t$ . The arrow length at  $x$  determines the likelihood that the electron will be found at  $x$ . More precisely, the modulus-squared of  $\Psi$ , which can be calculated with  $\Psi^* \Psi$ , is proportional to the probability density:

$$\rho(x) = \Psi^* \Psi \quad (9.1)$$

Given the electron is in some region  $A$  between  $x_1$  and  $x_2$ , the integral:

$$\alpha = \int_{x_1}^{x_2} \Psi^* \Psi dx$$

is *proportional* to the probability of finding the electron in  $A$ .

Recall that the product of a complex number and its own complex conjugate is a real number, and here we are doing  $\Psi(x)^* \Psi(x)$ , using the single complex value at position  $x$ , so the result will be real. But the complex conjugate is not a general purpose magic way to get a real number from a product of any two complex numbers;  $\Psi(x_1)^* \Psi(x_2)$  need not be real.

If we compute the same integral  $\beta$  for some larger surrounding region  $B$ , we can compute the conditional probability:

$$P(A|B) = \frac{\alpha}{\beta}$$

That is: the probability of finding the electron in  $A$  *given that* it is somewhere in  $B$  is given by the fraction  $\alpha/\beta$ .

If  $\Psi$  is suitably behaved (square-integrable; roughly, it goes to zero at some distance and does not become infinite anywhere) then we can compute the integral over the whole of our one dimension of space:

$$\alpha = \int_{-\infty}^{+\infty} \Psi^* \Psi dx$$

We can then include a factor of  $1/\sqrt{\alpha}$  within  $\Psi$  to "normalise" it, such that integrating the normalised  $\Psi^* \Psi$  over some region will directly give us the absolute (unconditional) probability of finding the electron in that region.

Some interesting things to note at this early stage:

- For the simple first example of the free electron with definite momentum, normalisation is not possible because the integral over all of space does not converge on a finite value.
- A global change in the amplitude of the function (scaling the entire function by some complex constant) is not a physically significant change; there is a set of wave functions  $a\Psi$  for any complex constant  $a$ , which all mean the same thing. What matters is how the amplitude varies from place to place (the same will turn out to be true for the complex phase).
- To normalise, we have to find the sum over all space of the mod-squared wave function. Interpreting the wave function as a vector, we're taking the inner product of the vector with itself, so we are in a sense finding the "length"-squared of the wave function as a vector. We then can then use this factor to scale it to be a unit vector, but preserving the relative shape of the wave (that is, preserving the "alignment" of the vector).

## 9.7 Schrödinger Equation

Any wave can be described as a sum of many simple component waves. (It is interesting that we use the word "component"; they are also basis vectors, so in vector terminology we should use the word component to refer to the complex constant factor applied to each simple wave included in the sum).

Each individual component wave has *two* parameters:

- if we nominate a fixed point in space, there is a frequency of oscillation,  $\nu$
- if we freeze time, we can measure the wavelength,  $\lambda$ , the distance between adjacent peaks in space



These can be independently adjusted (do not be confused by the familiar example of EM waves, where wavelength and frequency are coupled due to the constant speed of light!)

So the component wave can be described by the complex exponential:

$$\Psi(x, t) = \exp \left[ 2\pi i \left( \frac{x}{\lambda} - \nu t \right) \right]$$

Pick any fixed point in space, so  $x$  is constant, and  $\nu$  determines the rate of oscillation. Pick a fixed instant in time, so  $t$  is constant, and  $\lambda$  determines the distance between peaks. With both in play, we have a corkscrew complex wave pattern that is moving.

Anything we figure out for this model wave can be taken to be true for any linear combination of many such waves, in the sense that we can imagine decomposing some messy wave into a set of components, each component characterised only by two numbers.

Planck inferred the relationship between frequency and energy:

$$\nu = \frac{E}{h}$$

And de Broglie likewise for momentum and wavelength:

$$\lambda = \frac{h}{p}$$

So we can write the wave function very neatly in terms of energy and momentum instead:

$$\Psi(x, t) = \exp \left[ \frac{i(px - Et)}{\hbar} \right]$$

Nothing much has changed: as before, we have two parameters shaping a complex corkscrew wave. (We use  $\hbar = h/2\pi$  for brevity because that combination isn't going away.) All that has changed is that we've got two parameters with a physical interpretation for something we've previously thought of as a "particle".

We can take the partial differential of the above w.r.t  $t$  or  $x$ , and the way that works with exponentials is strangely illuminating.

Doing  $t$  first:

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \exp \left[ \frac{i(px - Et)}{\hbar} \right]$$

The constant factor is copied outside the exponential, which otherwise remains the same. So in fact:

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi$$

We can tidy up by multiplying both sides by  $i\hbar$ :

$$i\hbar \frac{\partial \Psi}{\partial t} = E\Psi$$

The exact same procedure with  $x$  yields:

$$-i\hbar \frac{\partial \Psi}{\partial x} = p\Psi$$

But we can also take the second derivative and get:

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = p^2 \Psi$$

Returning to our physical interpretation, a free particle has energy that is purely kinetic, related to its momentum by:

$$p^2 = 2mE$$

(This is just  $\frac{1}{2}mv^2$  smushed into the definition of momentum,  $mv$ .)

Substituting the Planck and de Broglie relations:

$$\frac{\hbar}{2m} = \lambda^2 \nu$$

In general a corkscrew wave is governed by two independent parameters:

- momentum, which goes with wavelength (and the  $x$  coordinate)
- energy, which goes with frequency (and the  $t$  coordinate)

We've now coupled them, making them no longer independent. But we've also added a new parameter: the particle's mass. For a free particle of a given mass, if you know the momentum you know the energy, and vice versa. Equivalently, if you know the wavelength you know the frequency, and vice versa.

Returning to the classical relationship between momentum, energy and mass, we can use it to rewrite our expression for  $p^2\Psi$ , substituting into the R.H.S. to easily obtain:

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = 2mE\Psi$$

And as we also have an expression for  $E\Psi$ , let's isolate that:

$$E\Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

and insert our  $E\Psi$  expression:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

So, recalling that  $\Psi$  is an abbreviation for  $\Psi(x, t)$ , a complex valued function of space and time, now we have a differential equation that relates only these things:

- $\hbar$ , Planck's constant, a universal fixed real number with units of joules-seconds, very accurately determined by experiment, not something we can adjust to fit this equation to different scenarios
- $i$ , which just provides a 90° phase shift
- the first partial derivative of  $\Psi$  w.r.t. to time, which is another function of space and time that tells you how  $\Psi$  is changing
- $m$ , the mass of the particle
- the second partial derivative of  $\Psi$  w.r.t. space.

This means that from a snapshot  $\psi$  (at a specific instant of time) of the wave function of a particle with a known mass, so you have its shape in space, you can find the second derivative of that shape w.r.t. space, then multiply that by  $i\hbar/2m$  and you have the the first partial derivative of  $\Psi$  w.r.t. to time. That is, a snapshot contains complete information about the past and future of the wave; it tells you how to compute every past and future state.

So far, so kind-of rigorous. The situation becomes vaguer when we introduce a force field acting on the particle.

Schrödinger himself seems to have mostly taken a guess and found that the resulting equation agreed with several previously unexplained experimental results. Many widely used textbooks don't even give any background for it but merely state it. More advanced theory can be used to derive it, e.g. it is a low-energy approximation of QED.

The full classical account of the energy of a particle is:

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

where the potential is a function  $V(x)$ . Realistically it will also be a function of  $t$ , but later we're going to pretend it isn't.

Some authors note that by multiplying the above throughout by  $\Psi$ :

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

we obtain some scaffolding into which we can plug in our expressions for  $E\Psi$  and  $p^2\Psi$ :

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (9.2)$$

And this is the same as the free particle equation with the added  $V\Psi$  term, and is the complete Schrödinger equation which governs the time evolution of  $\Psi$ .

The extra term doesn't change the important property that if you have a snapshot  $\psi(x)$  taken of  $\Psi(x, t)$  at a specific initial instant of time, then you know all future states (glossing over what happens when there is any kind of interaction, including measurements).

This is sometimes contrasted with Newton's 2nd law relating acceleration to force, acceleration being the second order derivative of the position w.r.t time. Each time we integrate we need to conjure up a constant of integration, and we have to integrate acceleration twice to get the position. The two constants we need to add are the position and velocity. Thus a snapshot of the position of a particle is not generally enough to know what is happening to it.

But a snapshot  $\psi(x)$  taken of  $\Psi(x, t)$  at some time is not just one number, but a continuous function giving a (complex) number at each point  $x$  along the line, so it is generously endowed with information. If we decompose the snapshot into component waves, each one has its own wavelength.

And if we multiple  $\Psi$  by some constant (possibly complex) factor, the result is still a solution to the function. Such arbitrary constant scale factors make no difference to the physical meaning; what matters is how the function varies from location to location (and from time to time). This is what allows us to normalise the function (where possible) to ensure that it sums to 1 over all of space.

## 9.8 Time Evolution

We can say little here about wave functions unless they can be normalised, i.e. wave functions that tend to zero at infinity. Assuming this is the case, if we integrate the PDF over all of space:

$$\int_{-\infty}^{+\infty} \Psi^* \Psi \, dx$$

we expect the result to be constant (if normalised, it should always remain 1 as time passes), i.e.

$$\frac{d}{dt} \int_{-\infty}^{+\infty} \Psi^* \Psi \, dx = 0$$

Note that as we are integrating over  $x$ , outside the integral  $x$  is not a variable. We can move the differentiation w.r.t.  $t$  inside the integral, but only we change it to partial, because inside the integral  $x$  is a variable:

$$\int_{-\infty}^{+\infty} \frac{\partial}{\partial t} \Psi^* \Psi \, dx = 0$$

Focusing on the inside of the integral, by the product rule:

$$\frac{\partial}{\partial t} \Psi^* \Psi = \frac{\partial \Psi^*}{\partial t} \Psi + \frac{\partial \Psi}{\partial t} \Psi^*$$

Now, the Schrödinger equation gives us an expression for the partial time derivative of the wave function by slightly rearranging (9.2):

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{iV}{\hbar} \Psi$$

From this we can get the same for the complex conjugate:

$$\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{iV}{\hbar} \Psi^*$$

Plugging those into our expression:

$$\frac{\partial}{\partial t} \Psi^* \Psi = \left[ -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{iV}{\hbar} \Psi^* \right] \Psi + \left[ \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{iV}{\hbar} \Psi \right] \Psi^*$$

Multiplying out:

$$\frac{\partial}{\partial t} \Psi^* \Psi = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} \Psi + \frac{iV}{\hbar} \Psi^* \Psi + \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} \Psi^* - \frac{iV}{\hbar} \Psi \Psi^*$$

The second and fourth terms cancel each other:

$$\frac{\partial}{\partial t} \Psi^* \Psi = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} \Psi + \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} \Psi^*$$

Also there's a common factor we can pull out:

$$\frac{\partial}{\partial t} \Psi^* \Psi = \frac{i\hbar}{2m} \left[ \frac{\partial^2 \Psi}{\partial x^2} \Psi^* - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right]$$

Recall that we are working out an expression for this because it appears inside an integral over all space:

$$\int_{-\infty}^{+\infty} \frac{i\hbar}{2m} \left[ \frac{\partial^2 \Psi}{\partial x^2} \Psi^* - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right] dx$$

Now the fundamental theorem of calculus is that integration is the inverse of differentiation, so there is clearly some redundancy here in that we are taking the second partial differential w.r.t.  $x$  only to then integrate over all  $x$ .

To make this explicit:

$$\frac{\partial}{\partial t} \Psi^* \Psi = \frac{i\hbar}{2m} \left[ \frac{\partial}{\partial x} \left( \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right] \quad (9.3)$$

The integral and the partial differentiation w.r.t.  $x$  cancel out to give us an expression that we can evaluate at the two limits and take the difference:

$$\frac{d}{dt} \int_{-\infty}^{+\infty} \Psi^* \Psi dx = \frac{i\hbar}{2m} \left[ \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right] \Big|_{-\infty}^{+\infty}$$

If we do that, we will have an expression for the rate of change, w.r.t. to time, of the integral of  $\Psi^* \Psi$  over all space.

But at these limits, we've said  $\Psi$  goes to zero, so as to be normalisable, making the whole expression zero at those limits. So in fact we've shown that, as we wanted:

$$\frac{d}{dt} \int_{-\infty}^{+\infty} \Psi^* \Psi dx = 0$$

So if it is possible to normalise a wave function at all, and it satisfies (9.2), then the constant of normalisation lives up to its name: it is the same for all time.

## 9.9 Motion

Given this abstract notion of an electron being entirely represented by a complex-valued function of position, how can we make sense of an electron moving?

Supposing the wave function is more concentrated in some region, it makes sense to compute the expectation value of the position variable:

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x) dx$$

Substituting our definition of  $\rho$  from (9.1):

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \Psi^* \Psi dx$$

remembering always that  $\Psi$  is short for  $\Psi(x, t)$ , so  $\langle x \rangle$  is also a function of  $t$ , and so this gives us a way of thinking about motion: the way the expectation value of the position changes with time.

$$\frac{d}{dt} \langle x \rangle = \frac{d}{dt} \int_{-\infty}^{+\infty} x \Psi^* \Psi dx$$

We can rearrange to move the derivative inside the integral, giving:

$$\frac{d}{dt} \langle x \rangle = \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t} \Psi^* \Psi dx$$

Like before, it's the  $t$ -derivative of something that depends on  $x$ , inside the integral over  $x$  we clarify that it is the partial derivative, and therefore  $x$  is a constant for that derivative.

And borrowing from (9.3) we can rewrite this as:

$$\frac{d}{dt} \langle x \rangle = \frac{i\hbar}{2m} \int_{-\infty}^{+\infty} x \frac{\partial}{\partial x} \left( \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx$$

This isn't as simple as before where we cancelled out the integration and the differentiation, because of the pesky  $x$ . But the good news is this is the easiest ever opportunity for integration by parts. Recall:

$$\int u \frac{dv}{dx} dx = uv - \int v \frac{du}{dx} dx$$

So  $u$  is just  $x$  and to get  $v$  we have to calculate it at the limits:

$$v = \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \Big|_{-\infty}^{+\infty}$$

Plugging them in:

$$x \left( \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right) \Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \left( \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right) \frac{dx}{dx} dx$$

As before, with  $\Psi$  vanishing at infinity the first term can be removed, and of course  $dx/dx$  is 1. Finally the above is just the integral from our  $\langle x \rangle$  expression, so:

$$\frac{d}{dt} \langle x \rangle = -\frac{i\hbar}{2m} \int_{-\infty}^{+\infty} \left( \frac{\partial \Psi}{\partial x} \Psi^* - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx$$

Having unwrapped one layer with integration by parts we can pull the same trick with  $\frac{\partial \Psi^*}{\partial x} \Psi$ , with  $u = \Psi$  and  $v = \Psi^*$ , which once again means the  $uv$  term is zero, leaving:

$$- \int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \Psi^* dx$$

So putting this back into  $\langle x \rangle$ :

$$\frac{d}{dt} \langle x \rangle = -\frac{i\hbar}{2m} \int_{-\infty}^{+\infty} \left( \frac{\partial \Psi}{\partial x} \Psi^* + \frac{\partial \Psi}{\partial x} \Psi^* \right) dx$$

The two identical terms cancel with the 2 on the bottom of the fraction, so:

$$\frac{d}{dt} \langle x \rangle = -\frac{i\hbar}{m} \int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \Psi^* dx$$

If we think of the rate of change of  $\langle x \rangle$  as the expectation value of the velocity, or  $\langle v \rangle$ , we can multiply by  $m$  to get  $\langle p \rangle$ , which actually cancels the  $m$ .

$$\langle p \rangle = -i\hbar \int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \Psi^* dx$$



## 9.10 Operators Again

Another way to look at what we're doing here is discovering operators. To apply an operator  $\hat{O}$  and get its expectation value  $\langle O \rangle$ , the recipe is:

$$\langle O \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{O} \Psi dx$$

How does this relate to our previous discussion about observable operators (§9.5)? We said that the operator for an observable has orthogonal eigenvectors, with eigenvalues that are the value that will be measured. Our wave function at an instant in time  $\psi(x)$  is a vector. To get a coordinate from that vector, we evaluate the function for some position  $x$ , and so the vector has a coordinate for every point in space. Therefore it is a vector expressed in the "position basis".

If the particle is very precisely localised, the function's value (the coordinates) will be zero everywhere except at that precise location. At the theoretical extreme, it will be zero everywhere except at an infinitesimal single position (§8.2). That is, it will be a basis vector in the position basis.

An observable operator has to scale its eigenvectors by the value that would be measured for a state equal to that eigenvector. That is exactly what happens if we multiply  $\psi(x)$  by  $x$ : if it is a pure spike (a complex value of modulus 1) at some position  $x_1$ , and zero everywhere else, the spike (and thus the whole vector) will be scaled by the value  $x_1$ . Whereas if it isn't a pure spike (not a position eigenvector), each non-zero value will be multiplied by a different value (its own position value), which will distort the shape of the function (or equivalently, change the "direction" of the vector).

We also mentioned in passing that if we apply an observable's operator to a specific state vector, we get an adjusted vector, and if we take the inner product between the original state vector and the adjusted vector, the resulting scalar value will be the expectation value of the observable. And that is exactly what we are doing in the above integral:

$$\langle O \rangle = \langle \Psi | \hat{O} | \Psi \rangle$$

Because  $\Psi$  is a function of  $x$  and  $t$ , by integrating over all  $x$  we get a function of time, telling us the evolving expectation value of whatever observable the operator represents. This "operator sandwich" pattern is intuitively sensible when we apply the position operator to a wave function of position, because this fits precisely with how we understand the expectation value to be computed: it is the sum of every possible value multiplied by its probability of occurring.  $\hat{x}|\psi\rangle$  is just  $x\psi(x)$ . If we multiply that by  $\psi(x)^*$  then it will be  $x$  multiplied by the

probability of measuring the position to be  $x$ ; clearly then the integral over all space will be the expectation value  $\langle x \rangle$ .

So the position operator  $\hat{x}$  is just  $x$  itself:

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{x} \Psi dx = \int_{-\infty}^{+\infty} \Psi^* x \Psi dx$$

The momentum operator  $\hat{p}$ , which we discovered above by looking for the expectation value of momentum, is  $-i\hbar \frac{\partial}{\partial x}$ :

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{p} \Psi dx = \int_{-\infty}^{+\infty} \Psi^* (-i\hbar \frac{\partial}{\partial x}) \Psi dx = -i\hbar \int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

Compared to the position operator, it is somewhat less obvious what the momentum operator is doing to produce an expectation value for momentum. The intuitive process would be to sum (over all possible momenta) the product of each momentum and its probability of being measured. That would seem to require a wave function of momentum instead of position, and an integral over all momenta. And yet here we still have an integral over all positions, involving a wave function of position. *We have not yet changed basis.*

It is perhaps easier to comprehend this intuitively through the analogy with regular vectors, and by remembering that vectors are basis independent objects (§3.1). The observable operator acts on the state vector, in general changing both its length and alignment (unless the state vector happens to already be an eigenstate of the observable, in which case only the length changes). But this action would be the same regardless of the basis we are working in, and so it isn't necessary to get hung up on that point. Likewise, projecting the operated-on vector back on to the original state vector, to produce a scalar expectation value, is a geometrical, basis-independent operation. The inner product depends on the relative lengths and the angle between the two vectors. As long as when we change basis we do so in a way that preserves the inner product (that is, by a *unitary* operator), then the choice of basis is physically irrelevant.

Therefore, in this recipe for the expectation value, the operator  $\hat{O}$ , the state vector  $|\Psi\rangle$  and the adjusted vector  $\hat{O}|\Psi\rangle$  should all be understood as having an independent existence from any choice of basis:

$$\langle \Psi | \hat{O} | \Psi \rangle$$

That expression is a scalar value, and is the same regardless of the basis we work in. When we want to calculate it, we use the same basis throughout.

On the other hand, the expectation value is a meagre summary of the rich information available in state vector, so we shall retain our obsession with finding a way to change basis.

## 9.11 Time Independent Potentials

In the Schrödinger equation, if the potential  $V$  is constant everywhere (and thus may as well be zero everywhere), it reduces to the free particle equation that fell out automatically from the fact that kinetic energy is tied to momentum. If you know the energy, you know the momentum and vice versa, which means that if you know the shape of a time-independent snapshot of the wave  $\psi(x)$ , then you know everything.

If the potential is a function it gets trickier. To understand the effect of varying  $t$  and  $x$  separately, we can suppose the existence of two functions  $\psi(x)$  and  $\phi(t)$  that when multiplied give us  $\Psi(x, t)$ .

It is not generally true that this is possible. Even something as simple as  $\Psi(x, t) = x + t$  can't be separated into a product of two functions of  $x$  and  $t$ . It's obviously true that solutions to the zero-potential Schrödinger equation can be separated, simply because we obtained it from the assumption:

$$\Psi(x, t) = \exp \left[ \frac{i(px - Et)}{\hbar} \right]$$

which can easily be written as the product of two separate functions of  $x$  and  $t$ :

$$= \exp \left[ \frac{ipx}{\hbar} \right] \exp \left[ \frac{-iEt}{\hbar} \right]$$

But when a potential is included it transpires that we can only use separation of variables if the potential is only a function of  $x$ , not  $t$ . But we can still discover some useful things.

$$\Psi(x, t) = \psi(x)\phi(t)$$

Taking partials becomes ordinary differentiation, because the other factor is constant:

$$\frac{\partial \Psi}{\partial t} = \psi \frac{d\phi}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} \phi$$

So we just plug those into (9.2):

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

Dividing by  $\psi\phi$ :

$$i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \frac{1}{\psi} + V$$

To make this explicit, let's put the parameters on each function:

$$i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} \frac{1}{\psi(x)} + V(x)$$

The LHS only depends on  $t$ , the RHS only depends on  $x$ . This means if we hold  $x$  constant, and therefore the RHS constant, this equation still holds even if we vary  $t$ ! And of course vice versa. Which means both sides are equal to the same constant, which we will call  $E$  for a good reason (spoilers!)

Equating the LHS with  $E$ :

$$i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = E \therefore \frac{d\phi}{dt} = -\frac{Ei}{\hbar} \phi \therefore \phi = e^{-iEt/\hbar}$$

The RHS isn't so neat, but:

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V = E \therefore -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

Solutions for  $\psi$  will depend on  $V$  of course. But the whole wave function is therefore:

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$$

Why is this interesting? Because the more complicated space-sensitive part is frozen w.r.t. time, we can understand the time evolution by just looking at the extremely simple factor:

$$e^{-iEt/\hbar}$$

Whatever the solution to  $\psi$ , the complex value of every point in space is only changing by the above factor as time passes.

And that factor is really just  $e^{i\theta}$  with the angle being  $-Et/\hbar$ , so we know the modulus of the value isn't changing; it's just going "round and round" clockwise in the complex plane.

And if the modulus isn't changing, the probability density isn't changing, so the particle isn't moving. Hence solutions of this type are known as *stationary states*. The expectation value of the position is fixed, and so all other observables' expectation values are also constant, including energy.

When we constructed the Schrödinger equation (9.2) we did so by building an expression for the total energy in terms of the particle's kinetic energy and a potential:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Comparing this to our RHS differential equation:

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

So in one of these stationary states,  $\psi$  substitutes for  $\Psi$ , but otherwise it's the same. We can extract an operator for the energy (the Hamiltonian):

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V$$

And in a stationary state, it's just:

$$\hat{H}\psi = E\psi$$

This is an eigenvalue equation: for some solutions  $\psi$ , the  $\hat{H}$  operator has the same effect as multiplying by a constant, the energy eigenvalue  $E$  for that  $\psi$ . Another example that fits the vector-based framework for quantum mechanics that we began with.

All this is only true for the stationary states of separable  $\Psi(x, t)$  wave functions, but we can sum an infinite set of them to get other shapes:

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

So for each  $n$  there's a complex constant  $c_n$  to go with the stationary state  $\psi_n$  and an energy level  $E_n$  that controls how fast the global phase shift goes round and round.

Because we're adding complex values at each point in space, even though those component values each have a time-independent modulus, the sum of them does not. So this is a way to make non-stationary solutions. Wave packets that "move" can be composed by summing stationary states that do not. A particle confined inside a potential can be in a stationary state, or it can "slosh" from side to side in a complicated way due to being a linear combination of many such states.

## 9.12 Wave Functions as Vectors

For stationary states  $m$  and  $n$ :

$$\int \psi_m^* \psi_n dx = \delta_{nm}$$

This does not mean that  $\psi_m^* \psi_n$  is zero everywhere if  $m \neq n$ , but it does mean that for every non-zero value pointing in some direction in the complex plane, there's another value of the same modulus pointing the opposite way, to balance it out.

The above is a way of defining the inner product between two stationary states, and of showing that they are like orthogonal vectors in a complex vector space for that product.

In fact we can define our vector space for QM in two ways:

- as an uncountable continuum of *scattering states*
- As a countable infinity of *bound states*

### 9.12.1 Scattering States

In the uncountable case of scattering states, the vector is a function of a continuous coordinate and cannot be reduced to anything more compact than that. This happens when the potential is absent and we have a physical state that moves freely through space as a pulse waveform. The inner product is defined by an integral:

$$\langle \alpha | \beta \rangle = \int \alpha^* \beta dx$$

If we knew a particle's exact location,  $\alpha$ , our wave function of space  $\psi(x)$  would have a single spike where  $x = \alpha$  and be zero everywhere else. Alternatively if knew its exact momentum (and  $p = h/\lambda$ ) our wave function would be a wave with a single wavelength. So we're dealing with Fourier transforms. At these extremes of certainty/uncertainty, one domain has a simple wave of infinite extent, and the other domain has a spike representing that wave. It works either way round.

Thus far we've been working in "position space", using functions of  $x$ , but alternatively we could work in "momentum space", where the functions are  $\phi(p)$ . If we knew a particle's exact momentum,  $\phi(p)$  would be a spike, whereas if we knew its exact position,  $\phi(p)$  would be a single-component wave.

Either way, the point is that the elements of our vector space are functions of a continuous variable (a real number), and the inner product has to be an integral over that continuous variable.

A theoretical free particle, being a perfectly periodic wave that extends to infinity, although it is a superposition of all possible position eigenstates, is on the other hand a pure eigenstate of both momentum and energy.

### 9.12.2 Bound States

In the countable case of bound states, a potential traps a particle and the measurable energies are quantised, the energy being the eigenvalue of the energy operator applied to the stationary state eigenfunction at that energy level.

The energy eigenfunctions serve as a set of basis vectors. Why? Because the energy operator is Hermitian (the equivalent of a symmetric matrix except with complex elements) which means that among its eigenvectors, any two corresponding to distinct eigenvalues will be orthogonal, and so each possible energy value is represented by an eigenvector. We can create a weighted sum of them to make any possible state. We can use those weightings as the components of a vector describing a state. That is, the state of the lowest energy level is a column vector of numbers where the first component is 1 and all the other components are 0.

There are two complications to this story:

- In some situations we find that multiple eigenvectors have the same eigenvalue, so we cannot infer the state vector from an energy measurement.
- We can't measure the energy with absolute precision anyway. No system ever really collapses so its state vector is known to be precisely one of the eigenvectors of whatever observable is being measured. It always remains a superposition to some extent.

The inner product of two vectors is the sum of the products of the components of the two vectors (taking care to always complex conjugate the first one):

$$\langle \alpha | \beta \rangle = \sum_i \alpha_i^* \beta_i$$

So once we've established the basis and computed the eigenvalues, we can construct states that are combinations of the eigenvectors and figure out the probability of obtaining a given energy by summing, rather than integrating.

## 9.13 Energy Degeneracy

Given two eigenvectors of an Hermitian operator, if they have different eigenvalues then they are orthogonal (intuitively they can't be colinear because a linear operator can't apply a different scaling to vectors that are colinear). But what about the converse? If they are orthogonal do they have different eigenvalues?

Given two eigenstates of the energy operator,  $\psi_1$  and  $\psi_2$ , when we apply the operator it just scales them each by their own eigenvalue:

$$\begin{aligned}\hat{E}\psi_1 &= E_1\psi_1 \\ \hat{E}\psi_2 &= E_2\psi_2\end{aligned}$$

If  $E_1 \neq E_2$ , the two states must be orthogonal. What if we sum the two states and apply the energy operator to the result? The operator is linear, so applying it to a sum of states is the same as applying it to the states separately and then summing the result:

$$\hat{E}(\psi_1 + \psi_2) = \hat{E}\psi_1 + \hat{E}\psi_2 = E_1\psi_1 + E_2\psi_2$$

So the result is a linear combination of the two states. If  $E_1 \neq E_2$ , this result is not some single constant  $E_3$  multiplied by the sum of the states:

$$\hat{E}(\psi_1 + \psi_2) \neq E_3(\psi_1 + \psi_2)$$

But if  $E_1 = E_2$ , then we can pull out a single constant (let's use  $E_1$ ):

$$\hat{E}(\psi_1 + \psi_2) = E_1(\psi_1 + \psi_2)$$

In other words, any two eigenstates with the same eigenvalue can be added to get a third eigenstate. Obviously this is also true for any linear combination using weightings  $a, b$ , simply because if  $\psi$  is an eigenstate then so is  $a\psi$ :

$$\hat{E}(a\psi_1 + b\psi_2) = \hat{E}a\psi_1 + \hat{E}b\psi_2 = E_1a\psi_1 + E_2b\psi_2 = E_1(a\psi_1 + b\psi_2)$$

So this is a subspace of the whole vector space, a set of eigenvectors with the same eigenvalue, known (inevitably) as an eigenspace. Any scalar multiple of an eigenvector is also an eigenvector, so the line along which an eigenvector lies is (though not often) called an eigendirection, and is the simplest eigenspace that can arise with a linear operator.

In the simple case of a symmetric matrix operating on the plane, it will pick out two orthogonal directions along which it will perform a pure scaling. It may stretch along one direction but squeeze the other. Any vectors colinear with these two directions will only be scaled, their directions unaffected, and thus are eigenvectors. All other vectors will be rotated, and so are not eigenvectors. The set of eigenvectors aligned with one of the directions will all have the same eigenvalue, and so they form an eigenspace.

In QM the magnitude of a state vector is not significant; we always normalise it to a unit vector anyway. Therefore it is truer to say that observable states are



represented by eigendirections, and in a given direction we nominate the unit vector to be *the* eigenstate in that direction.

But in the higher dimensional complex vector spaces of QM, some operators will have eigenspaces that are not mere lines, but are themselves multidimensional. That is, there will be a set of vectors that are eigenvectors sharing the same eigenvalue, among which we can find an orthonormal basis of 2 or more dimensions.

The operation of scaling equally in all directions is a trivial example where all vectors are eigenvectors, and all have the same eigenvalue (the scaling factor), so they are all in the same eigenspace, and we can select any  $N$  that are not colinear to use as a basis of the  $N$ -eigenspace. Suppose we're dealing with a three dimensional vector space, and we scale up by a factor of 1.5 along the  $x$  and  $y$  directions, but shrink by 0.5 along the  $z$  direction. A vector aligned with either the  $x$  or  $y$  direction will be an eigenvector under this scaling operation, with the eigenvalue 1.5. So this is degeneracy: orthogonal eigenvectors with the same eigenvalues, sharing a planar eigenspace that is a proper subset of the whole space.

So while we can say confidently that if two eigenvectors of an Hermitian operator have different eigenvalues then they are orthogonal, we cannot claim the converse: two orthogonal eigenvectors do not necessarily have different eigenvalues. In some circumstances they do, but not all. In particular, by classical intuition, the system of a weight on a string swinging back and forth has a total energy related to the weight's maximum displacement, but it can swing along any axis, so there is an infinite set of states with the same energy. So it is in QM. The inability in some situations to determine the state from the energy is known as degeneracy.

## 9.14 Fourier Transforms

A function  $\psi(x)$  can be constructed by summing a collection of simple component waves, each with a different amplitude  $A$  and wavelength, although we replace the latter with momentum  $p$ . So one component is  $Ae^{ipx}$ , and we can suppose the existence of a function  $\phi(p)$  that tells you the amplitude  $A$  for a given momentum. Then if we integrate over all momenta:

$$\psi(x) = \int \phi(p)e^{ipx} dp$$

This tells you the total amplitude of the wave at a given position. But it's also structurally equation (8.2), implying that we can do the reverse:

$$\phi(p) = \int \psi(x)e^{-ipx} dx$$

So we can flip between "position space" and "momentum space" descriptions of the same state without loss of information. We've got two different functions that describe that state, functions of different variables, with (in general) different shapes.

We've also said that in QM we apply operators to switch between vector representations of the same state, in order to get their complex components in the representation for the observable for which we want a probability distribution. So how does this work with the momentum operator?

Given a state described by position,  $\psi(x)$ , we can apply the momentum operator:

$$\hat{p}\psi(x) = -i\hbar \frac{\partial\psi(x)}{\partial x}$$

Suppose  $\psi(x)$  is a simple wave of amplitude  $A$  (the amplitude isn't yet relevant, and we have no way of normalising such a function, but it will play a role in a moment):

$$\psi(x) = Ae^{ipx/\hbar}$$

To differentiate an exponential we just multiply it by whatever factor is applied inside the exponential, in this case  $ip/\hbar$ :

$$\frac{\partial}{\partial x}\psi(x) = \frac{ip}{\hbar} Ae^{ipx/\hbar}$$

So applying the momentum operator in full:

$$\hat{p}\psi(x) = -i\hbar \frac{ip}{\hbar} Ae^{ipx/\hbar}$$

The  $\hbar$ s cancel, the  $i$ s become 1, so we're left with:

$$\hat{p}\psi(x) = pAe^{ipx/\hbar} = p\psi(x)$$

So it's an eigenvalue equation: the observable quantity  $p$  is the eigenvalue of the operator  $\hat{p}$ , and so therefore we know that our choice of  $\psi(x)$ , a corkscrew wave, was an eigenstate of the momentum operator (we've just confirmed that the momentum operator does its job). But while any  $\psi(x)$  might not be an eigenstate of momentum in this way, it will always be a linear combination of eigenstates of momentum. We just need a function  $\phi(p)$  that gives us the amplitude (replacing  $A$ ) contributed by every possible momentum  $p$ , and then we can integrate over all possible momenta to build the position wave function:

$$\psi(x) = \int \phi(p) e^{ipx/\hbar} dp$$

Differentiation is linear: we can perform it on each component wave and sum the results and this is equivalent to differentiating the sum of the components. So the steps we went through above can be performed with any composite wave too. However, we will not find a simple eigenvalue.

To make this explicit, let's make our position wave function from just two different momentum eigenstates:

$$\psi(x) = A_1 e^{ip_1 x/\hbar} + A_2 e^{ip_2 x/\hbar}$$

Applying the momentum operator:

$$\hat{p}\psi(x) = p_1 A_1 e^{ip_1 x/\hbar} + p_2 A_2 e^{ip_2 x/\hbar}$$

The two terms of  $\psi(x)$  have each been scaled by a different momentum value. Furthermore they have different wavelengths so will interfere messily. So evidently this is not an eigenvalue equation.

But the way we've defined  $\psi(x)$ , we know it has a certain spectrum: two spikes, at  $p_1$  and  $p_2$ , and nothing at any other momenta. So as a function of  $p$  we would say:

$$\phi(p) = A_1 \delta(p - p_1) + A_2 \delta(p - p_2)$$

Let's compare the above discussion with regular vectors. A vector  $\vec{v}$  in one basis has a set of coordinates in that basis,  $v_k$ . The vector can be constructed by multiplying each basis vector  $\vec{e}_k$  by the corresponding coordinate and summing:

$$\vec{v} = \sum_k \vec{e}_k v_k$$

But we can transform the coordinates  $v_k$  by using an operator described by a matrix  $O$ . The coordinates,  $u_j$ , still describe the same vector but in a different basis, and are given by the matrix multiplication  $Ov$ , which means producing the  $j$ th coordinate in the new basis by taking the dot product of the  $j$ th row of the matrix with the coordinates in the original basis, so here  $j$  is the index of the coordinate we are calculating and  $k$  remains the summation variable:

$$u_j = \sum_k O_{jk} v_k$$

In Dirac notation we can write the inner product between two vectors as  $\langle a|b\rangle$ . Supposing we wanted to obtain the first coordinate of our vector  $\vec{v}$ , we could write that as  $\langle 1|v\rangle$ . The L.H.S. is not the numeric value 1; we're just using that as a label for the basis vector  $\vec{e}_1$ .

If the vectors are functions of a real variable such as position, the inner product is the integral over all values of that variable. But the basis vectors are  $\delta$  spikes, the integral will just pick out the value at that position, and so it's the equivalent of simply evaluating the function at that position:

$$\langle x|\psi\rangle = \int_{-\infty}^{+\infty} \delta(x-y)\psi(y)dy = \psi(x)$$

So we see a kind of equivalence between the following:

- the index  $k$  becomes the position  $x$
- the column vector of coordinates  $v_k$  becomes the wave function  $\psi(x)$
- the basis vector  $\vec{e}_k$  is equivalent to the  $\delta$  function that gives us a spike we can position at any  $x$ , i.e. the position basis
- the index  $j$  becomes the momentum  $p$
- $u_j$  is the momentum function  $\phi(p)$

The tricky part is relating the matrix  $O$  to the position-space momentum operator  $\hat{p}$ .

Each row of a matrix can be viewed as a row vector, applied to the input column vector with the inner product to produce one coordinate of the output vector. For continuous functions, that would mean that we need to perform an integral to obtain one output "coordinate".

Using a matrix to convert to another basis means getting the coordinate for each basis vector in the new basis, which means taking inner product between the input vector and each basis vector. So each row of the matrix is just one basis vector of the new basis, but *expressed in the old basis*.

So to do this when converting from position basis to momentum basis, we need the set of functions that are the basis vectors of momentum *expressed in the position basis*, so then for any one such basis vector we can do the inner product between it and our input vector to find the "coordinate" (complex value) for some momentum.

As we've seen, the basis vector for momentum  $p$  expressed in the position basis is  $e^{-ipx}$ , a corkscrew wave, so the required inner product is simply:

$$\phi(p) = \int \psi(x)e^{-ipx}dx$$

## 9.15 Phase-space Formulation

Phase space is a conceptual space with both space and momentum dimensions. In the simplest case of motion in one spatial dimension, phase space has two dimensions, one each of space and momentum. Classically a harmonic oscillator traces out an ellipse in phase space, as it oscillates between zero displacement with maximum momentum, and then maximum displacement with zero momentum, back and forth (or in phase space, round and round). The two dimensions are not independent, because one is the derivative (or gradient) of the other.

There is a rarely used phase-space formulation of QM in which we characterise a system by a real scalar function of phase space, that is,  $f(x, p)$ . This function of both position and momentum is an alternative way to capture all the information in a complex wave function of *either* position or momentum. For a simple harmonic oscillator the form of the function is rigid and simply rotates in phase space as time passes, in a direct analogy with the classical time evolution.

## 9.16 Spin

Up to this point we've been mostly considering a specific application of the general model of QM, where the classical concepts of position and momentum, which are the building blocks for anything else we might measure, are represented as functions of a continuous variable. The function's value is a complex number that can be mod-squared to get the probability density of that variable. There is something intuitive about this in the space domain, which is why we start with that: it makes us think of an electron as being spread out through space, and having a density that varies. Only when some interaction occurs does it appear to be concentrated entirely at one point. But the momentum of the electron is modelled the same way, and this is not by itself very intuitive. It only becomes a little clearer when we realise that the space representation is a wave, and we can model waves as a sum of simple component waves with a set of frequencies. The momentum function is the Fourier transform of the position function.

But now we're going to consider intrinsic angular momentum. This is introduced to explain how electrons are deflected in a magnetic field, behaviour which is classically suggestive of the electron spinning around an axis, although that physical interpretation seems impossible because the electron's radius (if it is non-zero) is extremely small. Antipodal points on the surface of the electron would have to be moving relative to each other faster than the speed of light. Pauli suggested glossing over this question and just accepting that electrons have an intrinsic angular momentum that cannot be interpreted in some comfortable classical way.

## Chapter 10

# Relativity

Newtonian mechanics is based on the notion that the passage of time is universal, and objects have motions that determine how their positions change with the passage of time.

Einstein (and Minkowski) overturned this. Space and time are dimensions of a combined *spacetime*. The orientations of the space and time axes are a matter of perspective.

Rather than a point particle in space that is in motion, picture a path through spacetime, made up of points called *events*. The standard term for this is a *world line*, but I'm going to call it an *event path* (as it is not necessarily a line).

So in such a structure there is no motion at all; it is fixed and permanent.

Straight segments of an event path correspond to uniform (non-accelerated) motion. What we call acceleration is any curved portion of the path.

To assert that a particle is "at rest" during some straight segment of its event path is to choose to align the time axis with that segment. To assert that a particle is "in uniform motion" is to choose a time axis that is not aligned with the particle's path.

Any diagram of spacetime we draw, with a time axis and space axis, necessarily requires us to choose a specific alignment for the time axis, and thus a space axis that is (from the perspective of one at rest) orthogonal to it.

### 10.1 Clock Arrays, Spacetime Grids

Consider particles that only have one degree of freedom, i.e. they take positions along a line. Nominate an origin on the line. At the origin, place an emitter of a pulse of light, and on either side of it, stretching off to infinity, place

probes such that they are spaced one light-second away from their immediate neighbours.

Each probe contains a digital clock that measures elapsed seconds, but which is initially paused so its value does not advance as time passes. Each probe's paused clock displays an elapsed time that is equal to the probe's distance from the origin in light-seconds (note: we intentionally say the distance, which is always positive, not the displacement, which would be negative on the left and positive on the right).

At the origin, our emitter has a paused clock showing zero. It simultaneously emits the pulse of light and starts its own clock. When each probe detects the light pulse arriving, it starts its own clock.

In this way, we create a line of evenly spaced clocks that are synchronised with the origin's clock. We could now (if we wanted to) discard any notion of the distinct identity of each clock and treat them as an array of indistinguishable synchronised clocks. But instead we will label each clock with its displacement from the origin, so clocks on the left of the origin have increasingly negative labels, and those on the right have increasingly positive labels.

A spacetime diagram of this construction would be an orthogonal grid.

- The intersections of the grid represent events where a specific clock ticked forward to a new whole number of seconds
- Each vertical line connects all such events for a single clock, so a vertical line *is* a clock, in that it is the event path of a clock.
- Each horizontal line connects the events where a clock ticks forward to show a higher number of whole seconds have elapsed.

On such a diagram we can imagine our perception of time passing as being represented by a horizontal "line of simultaneity" that sweeps up through the grid.

## 10.2 Curved paths

A rogue particle is now introduced. It is free to move left or right on the line. It can accelerate freely. It is depicted on our spacetime grid by a curved path. On its journey it visits several of our clocks, which are able to sense when it passes very nearby and make a note of the time (according to that clock) when such a close encounter occurs. Thus we can build up a record of the movement of the particle, consisting of pairs of position (the clock's label) and time (the clock's time) captured at each clock it passes.

Because the rogue particle is outnumbered, it appears very clear that the the rogue is in non-uniform motion against the background of our original array of probes.

To even the score, suppose that rather than one such rogue particle, we have an array of them, spaced out along the line, and each having its own clock. These rogue clocks are synchronised by a light pulse just as before.

All the particles in the rogue array have been programmed to carry out a pre-determined sequence of accelerations, by firing little rocket thrusters. They all perform these accelerations in perfect unison and so remain the same distance from each of their neighbours. They are another co-moving array.

The result is that relative to each other, the rogue clocks are seemingly at rest, and could presume that it is our original array of clocks that are doing all the accelerating, and it being mere chance that their own rocket firings coincide perfectly with accelerations undertaken by other particles.

But nature is not fooled. At some basic level, the act of accelerating is accounted for and is an objective fact, not something that can be defined away by a change of perspective. The straight line segments of an event path are objectively straight, and the curved segments are objectively curved. The only valid conversions between points of view must be linear, in that they never convert a straight path into a curved path or vice versa.

So we have two fundamentally different arrays of co-moving particles, one in uniform motion and the other in accelerated motion.

Even so, we can imagine following the path of one rogue particle across space-time as its own clock ticks. Naively we might imagine rotating the diagram against our coordinate system as we trace the path, so as to keep the tangent to the path aligned with the time axis. After all, rotations are linear transformations that conserve the distance between each point and the centre of rotation. Each point moves in a circle around that centre.

The invariant separation between points is captured by the Pythagorean formula:

$$r^2 = t^2 + d^2$$

But the correct form of rotation to use between a space and a time coordinate is hyperbolic rotation, such that each point moves on a hyperbola as we rotate our perspective, and the equivalent of a distance between events being conserved is called the *interval*,  $s$ :

$$s^2 = t^2 - d^2$$

It transpires that the interval between events is an objectively real fact that all observers agree on. The absolute structure of the universe is *spacetime*, which is the set of all events, and all observers agree on the interval between any two events.



### 10.3 Spacetime Metric

We can define a metric, a way of taking the inner product of two vectors, and to find the squared length of a vector we take the inner product of the vector with itself. The metric for Euclidean geometry is the Kroneker delta,  $\delta$ , e.g. for three space dimensions:

$$\delta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

According to that metric, the squared length of vector  $\vec{v}$  in terms of its coordinates  $v^i$  is:

$$|\vec{v}|^2 = \sum_i \sum_j \delta_{ij} v_i v_j$$

As  $\delta$  picks out the terms where  $i = j$ :

$$|\vec{v}|^2 = (v_1)^2 + (v_2)^2 + (v_3)^2$$

This is the familiar theorem of Pythagorus.

But to find the interval between two events in spacetime, we need to use a different metric,  $\eta$  (eta). Now our indices  $i, j$  can take four values, traditionally given as 0, 1, 2, 3, with time being 0. So with a time dimension in addition to the three space dimensions, the correct metric happens to be:

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

where  $c$  is the speed of light, a quantity with cosmic significance. In honour of this we can take as our unit of distance the light-second, so that  $c$  is 1.

> Note that the signature of the diagonal of  $\eta$  could just as well be  $(-, +, +, +)$  instead of  $(+, -, -, -)$ , and as with anything that makes no difference, debate has raged on for over a century.

Furthermore, as our particles only move along a straight line we only need one space dimension, so altogether the metric can be written as:

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

So we have arrive at the modified form of Pythagorus such that the interval,  $s$  between two events separated by a distance  $d$  and a time  $t$  is given by:

$$s^2 = t^2 - d^2$$

It would be quite misleading to continue to picture this as a right triangle with  $d$  and  $t$  as the orthogonal short sides and  $s$  as the hypotenuse, because  $s$  has to remain constant as  $d$  and  $t$  both increase, which is impossible if the  $d$  and  $t$  sides remain orthogonal.

## 10.4 Interval Related To Proper time

A clock that travels inertially between two events separated by interval  $s$  will measure the elapsed proper time  $\tau$ , but this is in fact identical to the interval:

$$\tau = s = \sqrt{t^2 - d^2}$$

This is obvious given that in its own coordinate system, it remains at coordinate zero, and so  $d = 0$  and hence:

$$\tau = s = t$$

This underscores the invariant, universal, unambiguous nature of the interval between two events. Two synchronised clocks departing from some event, and arriving at another via different "routes" through spacetime, may each show a different elapsed proper time, and each's proper time is a measure of the "length" of the path it took (the sum of all the infinitesimal segments of interval along that path.)

But due to the nature of the metric, with time and space coordinates making opposite-signed contributions to the sum, less straight paths require *less* time to elapse for the particle taking them. Thus the straight line path between the events (that which would be taken by a uniform motion) is the *slowest* path possible, in that a particle taking that path will see its own clock advance by a greater duration than that of any particle taking some otherwise curved path.

## 10.5 Lorentz Factor

Consider a clock-carrying particle  $P$  that is in uniform motion relative to an array of co-moving clocks,  $A_n$ . Two events are of significance:

- $P$  passes by  $A_0$  when both  $P$ 's and  $A_0$ 's clocks read  $t_0$
- $P$  passes by  $A_1$  when  $A_1$ 's clock reads  $t_1$ .

As measured in the  $A$  frame, the elapsed time  $t$  between the two events is:

$$t = t_1 - t_0$$

Also in  $A$  the distance between the two events is the distance between the clocks:

$$d = A_1 - A_0$$

And with these two values,  $A$  can compute the constant velocity of  $P$  during its journey:

$$v = d/t$$

But things look a little different from the perspective of  $P$ . A uniformly moving clock regards itself as being at rest, so the interval between the two events is accounted for entirely by the passing of time, and so the elapsed time according to  $P$  is equal to the interval of the path it takes.

We know that the interval is an invariant, objective fact about reality, not something that changes based on perspective, and we also know that it equals the time measured by a clock moving inertially between events. So using the values for  $d$  and  $t$  obtained in  $A$  we can correctly calculate the elapsed time measured by  $P$ :

$$\tau^2 = t^2 - d^2$$

Pulling out a factor of  $t^2$ :

$$\tau^2 = t^2 \left(1 - \frac{d^2}{t^2}\right)$$

We can abbreviate this by using  $A$ 's value for the velocity  $v = d/t$ :

$$\tau^2 = t^2(1 - v^2)$$

And unsquaring both sides:

$$\tau = t\sqrt{1 - v^2}$$

So the ratio that will convert the proper time  $\tau$  measured by  $P$  back to the time coordinate separation  $t$  as measured in  $A$  is:

$$\gamma = \frac{1}{\sqrt{1 - v^2}}$$

This  $\gamma$  is the Lorentz factor. Note that as  $v$  is based on a time value  $t$  in seconds and a distance value  $d$  in light-seconds, it is a fraction of the speed of light.

If it had the value 1, that would be light speed. But at that precise value,  $\gamma$  is undefined, due to the zero on the bottom of the fraction. The elapsed time for any journey taken by a photon is always zero, and so there is no way to relate times recorded by a photon to times recorded by an array of clocks (a photon is not a clock).

Furthermore, at velocities greater than 1 (faster than light), the value is defined but unfortunately is imaginary, due the square root of a negative value. The square of the interval between events travelled between by faster-than-light particles is negative, and so the interval, which is the elapsed time recorded by a clock carried by such a particle, is positive-imaginary.

## 10.6 Lorentz Transformations

Two observers  $\rho$  and  $\phi$  moving apart at speed  $v$  will label the same event with different spacetime coordinates:  $(t_\rho, x_\rho)$  and  $(t_\phi, x_\phi)$ .

To transform back and forth between these systems we need a pair of matrices, each the inverse of the other, such that these invariants are conserved:

- the interval between events
- the speed of light

Note that for any

$$\begin{bmatrix} \gamma & v\gamma \\ v\gamma & \gamma \end{bmatrix}^{-1} = \begin{bmatrix} \gamma & -v\gamma \\ -v\gamma & \gamma \end{bmatrix}$$

## 10.7 Energy and Momentum

The momentum is a vector, so in 3 dimensions of space it is a 3-vector and can be resolved into 3 scalar components once a suitable basis has been chosen.

The kinetic energy is a scalar. But both are observer dependent. A particle at rest relative to the observer has momentum that is the zero vector and kinetic energy zero. Should another particle collide with the one at rest and cause both particles to travel away in new directions and speeds, the total momentum vector and the total kinetic energy scalar will be the same before and after the collision, but the values of these quantities are different depending on the observer.

To another inertial observer moving relative to this scene, exactly the same conservation laws will be found to be obeyed, just with different numbers involved. The two observers will disagree over the momenta and energies of the specific particles, and also over the total energy and momentum, as summed separately over both particles.

As before we will take as our unit of distance the light-second, so the speed of light  $c$  is 1. In this unit system, energy and mass are fully equivalent, because the famous:

$$E = mc^2$$

becomes:

$$E = m$$

The total energy of a particle is its mass times the Lorentz factor  $\gamma$ :

$$\gamma = \frac{1}{\sqrt{1 - v^2}}$$

In our everyday experience,  $v$  is practically zero, as we're expressing it as a fraction of the speed of light, so almost all the energy of a particle is in its mass. The contribution from the kinetic energy is almost non-existent.

But again, this is a frame-dependent quantity, because a particle only has a defined velocity relative to some chosen inertial frame.

If we combine the components of the momentum 3-vector with the energy scalar (the total energy  $m\gamma$  discussed above), we get a 4-vector called the 4-momentum. As always in the Minkowski metric, the magnitudes of these objects are related by:

$$m^2 = E^2 - |\vec{p}|^2$$

So the 4-momentum has magnitude  $m$ , the energy is "temporal" and the 3-momentum is "spatial". Enjoy the symmetry with:

$$s^2 = t^2 - d^2$$

It's interesting that the momentum provides the three spatial components, while energy provides the remaining temporal component (and indeed this is the case: momentum conservation is due to translational symmetry in space, and energy conservation is due to translational symmetry in time.)

As we know that momentum and energy are separately conserved from the viewpoint of any inertial observer, we therefore know that the combined 4-momentum must also be conserved.

The four coordinates are resolved relative to a coordinate system. We had to choose an orientation for the three axes that make up our spatial basis, which is a slice of spacetime. One way to visualise it is to discard one of the space dimensions, so that space is a planar slice through in a 3D spacetime. A given inertial observer regards their spatial slice through spacetime as containing all the events happening "now", making it a "slice of simultaneity".

Each inertial observer will use different coordinates for the 4-momentum, not just because they have a free choice of spatial basis, but also because they each have an event path through spacetime that is momentarily in a specific direction. Each observer, assuming themselves to be at rest (at least instantaneously), regards their own event path as aligned with the time axis, and orthogonal to their slice of simultaneity.

But despite the coordinates of the 4-momentum being different, they describe the same vector in spacetime. That is, two observers stating the 4-momentum of the same particle will use different coordinates for the same 4-momentum. The vector itself can now at last be said to be conserved even under a change of coordinate systems. Everyone agrees on what the 4-momentum is geometrically, so we no longer have to qualify the law of conservation of momentum with caveats about a single frame of reference.

If we scale the 4-momentum by  $1/m$  (that is, in some coordinate system, if we divide all the components of the 4-momentum by the particle's intrinsic mass), we obtain the 4-velocity:

$$\vec{u} = \frac{\vec{p}}{m}$$

The magnitude of this vector is always  $c$  (or 1 in our simplified units), because the 4-momentum's magnitude is always  $mc$  (or  $m$ ). In other words, the only information really carried by the 4-velocity is a direction. We're only modelling a *direction* in spacetime and can ignore the magnitude as not physically significant.

This division by  $m$  is not meaningful for a massless particle such as a photon, which is why momentum is more fundamental than velocity, as momentum can be discussed for all particles regardless of whether they have mass. Yet it's interesting that a photon's 4-vector nevertheless has magnitude  $c$  (or 1), just as if it had a very small mass  $m$  that we could divide by.

The relationship between the components of the 4-velocity  $\vec{u}$  and familiar concepts is not as straightforward as for the 4-momentum. The spatial slice of  $\vec{u}$  points in the direction of motion (of course), as does the ordinary velocity  $\vec{v}$ . But their magnitudes,  $u$  and  $v$ , are different:

$$u = \gamma v$$

Where  $\gamma$  is the Lorentz factor again. As we noted above, there's an identical relationship between the total energy  $E$  and the intrinsic mass:

$$E = \gamma m$$

Starting with the familiar Euclidean metric:

$$r^2 = x^2 + y^2$$

We want to express this in terms of  $x$  and  $y$  in “first order” (that is, not squared). We can square-root both sides:

$$r = \sqrt{x^2 + y^2}$$

But it’s not distributive so we’re stuck on the RHS. Let’s assume there are some magical objects  $A$  and  $B$  such that:

$$r = Ax + By$$

Of course there will be suitable numerical values for  $A$  and  $B$  given some specific pair of  $x, y$  values but the challenge here is to find  $A$  and  $B$  for all possible  $x$  and  $y$ , producing the same value as the square root of the sum of their squares.

To find out more about them, we can square both sides:

$$r^2 = (Ax + By)^2$$

And we’ve defined  $r^2$  as the sum of the squares of  $x$  and  $y$ , so:

$$x^2 + y^2 = (Ax + By)^2$$

Multiplying out the RHS, it has four terms:

$$x^2 + y^2 = AAx^2 + ABxy + BAxy + BB y^2$$

Note that we’ve been careful not to assume  $A$  and  $B$  are commutative, as they are magical objects of a kind unknown to us so far (where as  $x$  and  $y$  are ordinary numbers).

And indeed, from the above we can see some obvious constraints on them by pairing up the terms with the LHS:

- $AA$  and  $BB$  must both be 1.
- $AB$  and  $BA$  must either both be zero, or have equal magnitude and opposite sign (anti-commutative).



The second one is worth emphasising: we cannot assume that  $AB$  and  $BA$  are both zero just because they don't appear in the LHS, only that they sum to zero. It's possible but not necessary for them each to be zero.

Note that the dot product of a unit vector with itself is 1, while the dot product of two orthogonal vectors is zero. It's no surprise these objects fit the bill, given that they are the two short sides of a right triangle, of which the sum is the vector lying on the hypotenuse. This is not quite right however:

$$r = \vec{i}x + \vec{j}y$$

because  $r$  is not a vector; we intended it to be the magnitude of a vector. We can fix the equation by introducing a unit vector  $\vec{h}$  in the direction of the hypotenuse, whatever that might be (it's of no interest to us as we're not doing trigonometry today):

$$\vec{h}r = \vec{i}x + \vec{j}y$$

$$(\vec{h}r)^2 = (\vec{i}x + \vec{j}y)^2$$

$$\vec{h}^2 r^2 = \vec{i}^2 x^2 + 2\vec{i}\vec{j}xy + \vec{j}^2 y^2$$

$$r^2 = x^2 + y^2$$

It's like we're saying that all scalars can be thought of as the length of some vector whose direction we don't presently care about. But as noted, we've just come full circle (or triangle).

We can also meet these requirements with matrices:

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

$$B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

So that:

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

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

which means:

$$BA = -AB$$

and:

$$AA = BB = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

Technically we're getting the identity matrix  $I$  instead of 1, so we've actually found that:

$$Ir = Ax + By$$

which is again close enough (this time we're saying that any apparently ordinary number can instead be thought of as the matrix you get from multiplying  $I$  by that number - a "scaled" identity matrix).

Not all situations are as simple as the Euclidean case. Consider Minkowski spacetime:

$$s^2 = t^2 - x^2$$

This defines the interval  $s$  as the time measured by a clock travelling inertially between two events that an inertial observer measures as being separated by time  $t$  and distance  $x$ . Suddenly we're taking the difference rather than the sum which complicates matters considerably. Repeating the above exercise to find an  $A$  and  $B$  such that:

$$s = At + Bx$$

and doing the same business of squaring both sides and substituting the definition on the left:

$$t^2 - x^2 = (At + Bx)^2$$

And multiplying out:

$$t^2 - x^2 = AAt^2 + ABtx + BA tx + BBx^2$$

So this time we require that:

- as before,  $AA$  must be 1.
- but now,  $BB$  must  $-1$ .
- as before,  $AB$  and  $BA$  must either both be zero, or have equal magnitude and opposite sign (anti-commutative).

It's like we need to be able to "program" the system in a general way to be able to produce the right behaviour. Using matrices gives us ample flexibility:

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

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

So that:

$$AB = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

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

$$BA = -AB$$

and:

$$AA = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$

but:

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

So all requirement met, we have matrices  $A$  and  $B$  such that:

$$Is = At + Bx$$

> Is this right? Does linearity mean that if the matrices meet the requirements then they work?

## Appendix A

# Greek Alphabet

This is the Greek alphabet. Why not memorise it?

Name	Lower	Upper
Alpha	$\alpha$	$A$
Beta	$\beta$	$B$
Gamma	$\gamma$	$\Gamma$
Delta	$\delta$	$\Delta$
Epsilon	$\epsilon$	$E$
Zeta	$\zeta$	$Z$
Eta	$\eta$	$H$
Theta	$\theta$	$\Theta$
Iota	$\iota$	$I$
Kappa	$\kappa$	$K$
Lambda	$\lambda$	$\Lambda$
Mu	$\mu$	$M$
Nu	$\nu$	$N$
Xi	$\xi$	$\Xi$
Omicron	$o$	$O$
Pi	$\pi$	$\Pi$
Rho	$\rho$	$R$
Sigma	$\sigma$	$\Sigma$
Tau	$\tau$	$T$
Upsilon	$\upsilon$	$\Upsilon$
Phi	$\phi$	$\Phi$
Chi	$\chi$	$\chi$
Psi	$\psi$	$\Psi$
Omega	$\omega$	$\Omega$