V. Dirac Notation - Analogies with vectors and matrices

Tutorial: *LibreText Physics*, Graeme Ackland, U. of Edinburg: 1.7: Dirac Notation - Analogies with vectors and matrices

Dirac notation is a shorthand for integrals, for example **the overlap** between **two wavefunctions** can be written

$$\langle\chi|\phi\rangle \quad \text{instead of} \quad \int\int\int \chi^*(\mathbf{r})\phi(\mathbf{r})d^3\mathbf{r}.$$

Note: $|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$ is a linear superposition in the discrete (rather than continuous) basis set $\{|n\rangle\}$.

(Where d^3r is the **scalar volume element**, sometimes called $r^2\sin\theta\, d\theta d\phi dr$, $dxdydz$, dV, or $d\tau$)

But also if we have a **complete set of orthonormal basis states *i***, the **overlap** is also the sum of the overlaps between each i and χ and ϕ

$$\langle\chi|\phi\rangle = \sum_i \langle\chi|i\rangle\langle i|\phi\rangle$$

A summation convention is also sometimes used, such that when a state symbol appears twice, first as a ket, then as a bra, it is assumed to be summed over a complete set of orthonormal basis states. The expression above is then further abbreviated to $\langle\chi|i\rangle\langle i|\phi\rangle$. This convention can be confusing.

Compare this with the **vector dot product formula:**

$$b\cdot a = b_x\cdot a_x + b_y\cdot a_y + b_z\cdot a_x = \sum_i\left[\left(b\cdot e_i\right)\cdot\left(e_i\cdot a\right)\right]$$

where $\mathbf{e_i}$ **are the unit vectors in x, y and z directions**. Just as any vector can be expressed as a linear combination of $\mathbf{e_i}$, so any quantum state can be expressed as **a linear combination of basis states i**. There are certain conditions on the basis states, e.g. they must be 'orthonormal' $\langle j|i\rangle=\delta_{ij}$ just as $e_i.e_j = \delta_{ij}$. Just as the three Cartesian vectors span a three dimensional space, so the many **basis states span a many-dimensional space**. In some cases (**e.g. Fourier expansions, hydrogen wavefunctions)** there are an **infinite number of basis states** which are therefore related to spanning an infinite-dimensional space. Mathematicians call these '**Hilbert spaces'**. Any state ϕ can thus be viewed as a vector in a multi-dimensional space, where **each dimension** corresponds to **one of the basis functions**. It is thus common to use the words eigenstate and eigenvector interchangeably to refer to $|\phi\rangle$ Even before the discovery of quantum mechanics, mathematicians had solved many of the problems in this area.

In Dirac notation we have **two quantities**, **the bra and the ket**, whereas in vector algebra we have only one, this is because there is not an exact analogy to commutation for Dirac brackets: $\langle\chi|\phi\rangle=\langle\phi|\chi\rangle^*$ includes taking a **complex conjugate**. Consider manipulating the bras and kets. We can write a vector in terms of its components thus

$$A = \sum_i\left[e_i\cdot\left(e_i\cdot A\right)\right]$$

where $(e_i.A)$ is the amount of $\mathbf{A}$ along the e_i axis; the components. The quantities on either side of the equation are not numbers but **vectors**. We can generate a whole algebra based on vectors. Likewise we can write a state thus: $|\phi\rangle = \sum |i\rangle\langle i|\phi\rangle$ where $\langle \mathbf{i}|\phi\rangle$ **is the amount of ϕ along the *i* basis state**; the components or expansion coefficients. The quantities on each side of this equation are not numbers but **functions**. ϕ is a normalized wavefunction iff $\sum |\langle \mathbf{i}|\phi\rangle|^2 = 1$. We can then generate a whole algebra based on bras and kets.

For any different complete sets of basis states i and j, we can write: $|\phi\rangle = \sum |j\rangle\langle j|\phi\rangle$, and $|\phi\rangle = \sum |i\rangle\langle i|\phi\rangle$. **Expansions in *i* and *j*** are called different **representations** of ϕ. This is very similar to using different coordinate systems: the bases i and j are **analogous to two sets of axes rotated with respect to one another**. We might choose complete set of wavefunctions as a representation which includes $\boldsymbol{\phi}$, just as we sometimes choose axes such that some special vector points along the z -axis.

Going even further, the expansion in a basis can be done for any $|\phi\rangle$, so we can dispense with $|\phi\rangle$ and write:

$$\mathbf{1} = \sum |\mathbf{i}\rangle\langle\mathbf{i}|, \text{ the unit operator}$$

All this means is that **in any equation** you can always proceed by breaking the states down into a z **complete, orthonormal set of basis functions.**

<u>Hilbert Space:</u> We can represent a qubit as a **<u>Two-Dimensional Complex Hilbert space,</u>** C^2. **A quantum state is a ray in Hilbert space.** The state of the qubit at any given time can be represented **by a vector** in this complex Hilbert space. A qubit system of say 100 qubits can handle 2^{100} states.
Relative phases of waveforms (states) are of fundamental importance for quantum algorithms in that they allow for constructive interference and destructive interference.
Qubits are abstract mathematical objects with certain specific properties.

With regard to QC, it should be noted that **Quantum Mechanics or Matrix Mechanics is not Quantum Physic**s. Rather, it is the **collection of mathematical tools used to analyze physical systems** which are, to the best of anyone's ability to test, known to behave according to the laws of quantum physics.

Just as a classical bit has a state – either 0 or 1, a qubit also has a state. Two possible states for a qubit are the states |0> and |1> , which correspond to the states 0 and 1 for a classical bit. Notation like '| >' is called the *Dirac notation*. The difference between bits and qubits is that **a qubit can be in a state other than |0> or |1>**. It is **also possible to form <u>linear combinations of states</u>**, often called **superpositions**:

$$|\Psi> = \alpha\,|0> + \beta\,|0>$$

In the Dirac notation, **the symbol identifying a vector** is written inside a 'ket', and looks like | a > . We denote the **dual vector** for a (defined later) with a 'bra', written as < a | . Then **inner vector products** will be written as 'bra-kets' (e.g. <a | b >). While bras and kets are both elements of vector spaces, they are **elements of different vector spaces**. The ket corresponds to the normal vectors while the **bra corresponds to a covector.** Kets are part of one vector space while **bras are part of the corresponding dual vector space.**

The numbers a and ß are complex numbers, although for many purposes not much is lost by thinking of them as real numbers. Put another way, the state of a qubit is a *vector in a **two-dimensional complex vector space***. The special states | 0 > and | 1 > are known as *computational basis states*, and form an ***orthonormal basis*** for this vector space. We can examine a bit to determine whether it is in the state 0 or 1. Rather remarkably, **we *cannot examine a qubit to determine its quantum state***, that is, the values of a and ß. Instead, quantum mechanics tells us that we can *only acquire much more restricted information* about the quantum state. When we measure a qubit we get either the result 0, with probability $|a|^2$, or the result 1, with probability $|ß|^2$. Naturally $|a|^2 + |ß|^2 = 1$, since the probabilities must sum to one. Thus, in general **a qubit's state is a *unit vector in a two-dimensional complex vector space***. This dichotomy between the unobservable state of a qubit and the observations we can make lies at the heart of quantum computation and quantum information. A qubit can **<u>exist in a continuum of states between |0> and |1></u>**, until it is observed. When a qubit is measured, it only ever gives '0' or '1' as the measurement result – probabilistically. **Because $|a|^2 + |ß|^2 = 1$**, we may write this as (**<u>See Section VIII</u>**.)

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right)$$

where **θ, ϕ and γ** are real numbers. We can ignore the phase factor of $e^{i\gamma}$ out the front, because it has no observable effects. The numbers θ and ϕ define a point on the unit three-dimensional complex sphere, as shown in Section V.

This sphere is often called the Bloch sphere; it provides a useful means of visualizing the state of a **single qubit**. How much information is represented by a qubit? Paradoxically, there are an infinite number of points on the unit sphere.

A **<u>bra-ket pair</u>** can be thought of as a **vector projection (i.e., a dot product)** - the projection of the content of the ket onto the content of the bra, or the "**shadow" the ket casts on the bra.** Example, ⟨Φ|ψ⟩ is projection of state ψ onto state Φ. It is the amplitude (probability amplitude) that a system in state |ψ⟩ will be subsequently found in state |Φ⟩

Suppose we have **two qubits**. **A two qubit system** has **four computational basis states** denoted $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$. A pair of qubits can also exist in superpositions of these four states, so the quantum state of two qubits involves associating a **complex coefficient, sometimes called an amplitude**, with each computational basis state, such that the state vector describing the two qubits is

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Important **2 bit states** are the 4 Bell states, e.g.: $\frac{|00\rangle + |11\rangle}{\sqrt{2}}$

Dirac notation is a succinct and powerful language for expressing quantum mechanical principles; in some of our examples that follow, restricting attention to one-dimensional examples reduces the possibility that mathematical complexity will stand in the way of understanding. Quantum Mechanics texts make extensive use of Dirac notation.

Wave-particle duality is the essential concept of quantum mechanics. In 1924 Louis De Broglie expressed this idea mathematically as λ = h/mv = h/p. On the left is the wave property , and on the right the particle property mv, its momentum. The most general **coordinate space wavefunction for a free particle with wavelength λ** is the complex Euler function shown below.

$$\langle x|\lambda\rangle = \exp\left(i2\pi\frac{x}{\lambda}\right) = \cos\left(2\pi\frac{x}{\lambda}\right) + i\sin\left(2\pi\frac{x}{\lambda}\right)$$

Feynman called this equation "*the most remarkable formula in mathematics*." He referred to it as "our jewel." And indeed it is, because when it is enriched with de Broglie's relation it serves as the **foundation of quantum mechanics**.

According to de Broglie's hypothesis, a particle with a well-defined wavelength also has a well-defined momentum. Therefore, we can obtain the momentum wavefunction (unnormalized) of the particle in coordinate space by substituting the deBroglie relation into Equation

$$\langle x|p\rangle = \exp\left(\frac{ipx}{\hbar}\right)$$

.Quantum mechanics teaches that **the wavefunction contains all the physical information about a system** that can be known, and that **one extracts information** from the wavefunction **using quantum mechanical operators**. There is, therefore, **an operator for each observable property.**

For example, in momentum space if a particle has a well-defined momentum we write its state as |p>. If we operate on this state with the momentum operator ^p, the following eigenvalue equation is satisfied.

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

We say the system is in a state which is an eigenfunction of the **momentum operator ^p** with **eigenvalue p**. In other words, operating on the momentum eigenfunction with the momentum operator, in momentum space, returns the **momentum eigenvalue times the original momentum eigenfunction**. From λ = h/mv = h/p λ ν

The state space in quantum mechanics is a complex finite or infinite vector space. Dirac denotes **an element *f* of the vector space** by $|f\rangle$, which he then calls a ket vector. An example for a one-dimensional ket is Schrödinger's wave function |ψ>, whose representation in position space is the well-known complex-valued wave function ψ(x) . An example for a four-dimensional ket is the vector

$$|\psi\rangle \overset{\text{def}}{=} \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

We then **define a dual** to each **ket** called the **bra**. We get a bra from the respective ket by taking its conjugate complex (if the ket is a vector, we also need to transpose):

$$\langle f| \overset{\text{def}}{=} (f^*)^\top = f^\dagger$$

Note that the **ket |ψ>** stands for the **entire wave function ψ**.

The scalar product of two vectors can then be written with the bra and the ket as

$$\langle f| \overset{\text{def}}{=} (f^*)^\top = f^\dagger$$

we then have

$$\langle f|g\rangle = \langle g|f\rangle^*$$