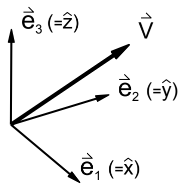
State vectors & Dirac brackets

Conventional vector notation. First look at *ordinary* 3D space, which is a vector space. Draw also three unit or basis vectors:



This vector can be expressed as

$$\vec{V} = a_1\,\vec{e}_1 + a_2\,\vec{e}_2 + a_3\,\vec{e}_3. \tag{1}$$

where the a_n's are vector components. We will add the extra detail to (1) that vectors can be multiplied by numbers from either side: $a_1\vec{e}_1$ and $\vec{e}_1 a_1$ mean the same thing, that $\vec{e}_1$ is multiplied by a_1. Using Σ,

$$\vec{V} = \sum_n a_n\,\vec{e}_n = \sum_n \vec{e}_n a_n. \tag{2}$$

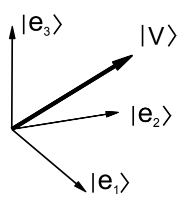
Using the dot products between the basis vectors $\vec{e}_1\cdot\vec{e}_1 = 1$, $\vec{e}_1\cdot\vec{e}_2 = 0$, and so forth, we can project out the components,

$$a_2 \;=\; \vec{e}_2\cdot\vec{V} \;=\; \vec{V}\cdot\vec{e}_2. \tag{3}$$

Instead of an arrow, we can use **Dirac brackets** for the ordinary vectors that have been described so far. we enclose vectors in a bracket,

$$\vec{V} \;\rightarrow\; |V\rangle$$

The word **ket** (part of "bracket") is another word for a vector. Basis vectors are also kets:



$$\vec{V} \;=\; a_1\,|e_1\rangle + a_2\,|e_2\rangle + a_3\,|e_3\rangle \;=\; \sum_n a_n\,|e_n\rangle. \tag{4}$$

We will project out components as in (3). But in Dirac notation **we do not write dot products**. Instead, for every ket or vector $|V\rangle$ we define a **dual vector** or **Hermitian conjugate** vector $\langle V|$. Specifically $\langle V|$ represents the **operation of taking a dot product** (or **dual product**):

$$\langle V| \;=\; \vec{V}\cdot, \qquad \langle V|U\rangle = \vec{V}\cdot\vec{U}$$

Problem 1. Explain the projecting-out of components

$$a_n \;=\; \langle e_n|V\rangle. \tag{5}$$

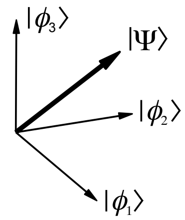
Problem 2. The **completeness relation** is one of the most important statements of the Dirac formalism:

$$\sum_n |e_n\rangle\langle e_n| \;=\; 1 \tag{6}$$

$$\Big(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| + |e_2\rangle\langle e_2| \;=\; 1\Big)$$

Prove it by acting with the left-hand side of (6) on a vector $|V\rangle$ to show (using (5)) that this does in fact just give back $|V\rangle$ itself.

Quantum mechanics is a vector space of states. You will often see the state of a system referred to not as a wave function $\Psi(x)$, but as a state vector $|\Psi\rangle$.



As for the $\vec{e}_n$'s and $|e_n\rangle$'s, $\langle\phi_n|\phi_m\rangle = \delta_{nm}$, i.e. 1 if $n=m$ and 0 if $n\neq m$. The state (or state vector, or ket) $|\Psi\rangle$ is now

$$|\Psi\rangle = a_1\,|\phi_1\rangle + a_2\,|\phi_2\rangle + a_3\,|\phi_3\rangle + \ldots \tag{7}$$

The dots mean there can be any number of basis vectors, even an infinite number. The projecting-out of components in $a_n = \langle\phi_n|\Psi\rangle$.

Whenever quantum mechanics takes the form of a Schrödinger equation (**not always the case!**) then each state vector in the Hilbert space corresponds to a particular wave function:

$$\text{State vector } |\Psi\rangle \;\Rightarrow\; \Psi(x) \;\text{ (wave function)}$$

and the "dot product" is the integral

$$\langle\Phi|\Psi\rangle \;=\; \int \Phi^*(x)\Psi(x)dx \tag{8}$$

For a **normalized** state $|\Psi\rangle$,

$$\langle\Psi|\Psi\rangle \;=\; \int \Psi^*(x)\Psi(x)dx \;=\; 1 \tag{9}$$

which as you know says that probability adds up to 1 over all x.

Problem 3. Show that the energy states in an infinite square well (of width L) are orthonormal, $\langle\phi_n|\phi_m\rangle = \delta_{nm}$.

The new aspect of vectors in quantum mechanics is that **its components can be complex**. In quantum mechanics these complex components are oftern called **amplitudes**. In Dirac notation we add one last rule: **Brackets in reverse order are complex-conjugates**. For example, Eq (5) is now replaced by

$$\langle\phi_2|\Psi\rangle = a_2, \quad \langle\Psi|\phi_2\rangle = a_2^*. \tag{10}$$

Problem 4. Explain (10) in terms of (8).

The vector space of quantum mechanics is called a Hilbert space. In Dirac notation, the **three central properties of a Hilbert space** are

$$\boxed{\begin{aligned} \langle\phi_n|\phi_m\rangle \;&= \delta_{nm} \quad (\textbf{Orthonormal basis})\\ \sum_n |\phi_n\rangle\langle\phi_n| \;&=\; 1 \quad (\textbf{Completeness})\\ \langle\phi|\psi\rangle \;&= \langle\psi|\phi\rangle^* \quad (\textbf{Complex space}) \end{aligned}}$$

Problem 5. Instead of an infinite square well, where the wave function must be zero at the end, consider a particle moving on a ring of total circumference L. If x is the position along the circumference, show that the Schrödinger wave functions

$$\phi_n(x) \;=\; \frac{1}{\sqrt{L}}\,e^{2\pi i n x/L}$$

(where n runs from $-\infty$ to $+\infty$, including zero) are orthonormal, $\langle\phi_n|\phi_m\rangle = \delta_{nm}$.

Problem 6. Suppose we have a state $|\Psi\rangle$ where the particle is localized uniformly on half the ring:

$$\Psi(x) \;=\; \begin{cases} \sqrt{2/L}, & 0 < x < L/2 \\ 0, & L/2 < x < L \end{cases}$$

(a) Check that this state is normalized. (b) What are the components a_n of $|\Psi\rangle$, using the basis states $|\phi_n\rangle$ given in Problem 5?

Problem 7. Insert the completeness relation to show that the product $\langle\Psi|\Psi\rangle$ of a vector/ket/state $|\Psi\rangle$ with itself is the sum of the squared *magnitudes* of its complex components:

$$\langle\Psi|\Psi\rangle = \sum_n |a_n|^2. \tag{11}$$

For a **normalized** state $|\Psi\rangle$, Eq (11) says

$$\langle\Psi|\Psi\rangle \;=\; \sum_n |a_n|^2 \;=\; 1 \tag{12}$$

This is another way to interpret normalization besides Eq (9). It says that for the state $|\Psi\rangle$ we can interpret each of its $|a_n|^2$ as the probability of finding the system in precisely state $|\phi_n\rangle$,

$$\text{Prob(state } n) \;=\; p_n \;=\; |a_n|^2.$$

Eq (12) says that these probabilities add up to 1 for all states, not just for all x as in Eq (9).

Problem 8. In Problem 6, what are the probabilities of finding the system to be exactly in the nth state $|\phi_n\rangle$? Do all of the probabilities add up to 1? Note the identity $\sum_{\text{all odd } n} 1/n^2 = \pi^2/4$. The sum over all odd n includes negatives. (Careful: Treat $n=0$ separately.)

Problem 9. Matrices. To show you understand matrices, make a clear drawing of the matrix operation that represents the equation

$$b_n \;=\; \sum_m M_{nm} a_m.$$

An operator $\hat{A}$ on a vector space (for example a quantum Hilbert space) turns one vector of the space into another:

$$|\Phi\rangle \;=\; \hat{A}|\Psi\rangle$$

In the following problem you show that $\hat{A}$ is doing a matrix multiplication on the components of the vector $|\Psi\rangle$.

Problem 10. Suppose the operator $\hat{A}$ on a vector space (for example a quantum Hilbert space) turns a vector $|\Psi\rangle = \sum a_n|\phi_n\rangle$ into another vector $|\Phi\rangle = \sum b_n|\phi_n\rangle$. Insert the completeness relation into two places on the right-hand side of $|\Phi\rangle = \hat{A}|\Psi\rangle$ to show that the action of $\hat{A}$ is a matrix operation relating a_n and b_n (viewed as column vectors), where the matrix elements are $A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle$.