

Dirac Notation

1 Vectors

1.1 Inner product

Recall from linear algebra: we can represent a vector V as a column vector; then $V^\dagger = (V^T)^*$ is a row vector, and the **inner product** (another name for dot product) between two vectors is written as

$$A^\dagger B = A_1^* B_1 + A_2^* B_2 + \dots \quad (1)$$

In conventional vector notation, the above is just $\vec{A}^* \cdot \vec{B}$. Note that the inner product of a vector with itself is positive definite; we can define the **norm** of a vector to be

$$|V| = \sqrt{V^\dagger V} \quad (2)$$

which is a non-negative real number. (In conventional vector notation, this is $|\vec{V}|$, which is the length of \vec{V}).

1.2 Basis vectors

We can expand a vector in a set of basis vectors $\{\hat{e}_i\}$, provided the set is **complete**, which means that the basis vectors span the whole vector space. The basis is called **orthonormal** if they satisfy

$$\hat{e}_i^\dagger \hat{e}_j = \delta_{ij} \quad (\text{orthonormality}), \quad (3)$$

and an orthonormal basis is complete if they satisfy

$$\sum_i \hat{e}_i \hat{e}_i^\dagger = \mathbf{I} \quad (\text{completeness}), \quad (4)$$

where \mathbf{I} is the unit matrix. (note that a column vector \hat{e}_i times a row vector \hat{e}_i^\dagger is a square matrix, following the usual definition of matrix multiplication).

Assuming we have a complete orthonormal basis, we can write

$$V = \mathbf{I}V = \sum_i \hat{e}_i \hat{e}_i^\dagger V \equiv \sum_i V_i \hat{e}_i, \quad V_i \equiv (\hat{e}_i^\dagger V). \quad (5)$$

The V_i are complex numbers; we say that V_i are the components of V in the $\{\hat{e}_i\}$ basis.

1.3 Eigenvectors as basis vectors

Sometimes it is convenient to choose as basis vectors the **eigenvectors** of a particular matrix. In quantum mechanics, measurable quantities correspond to hermitian operators; so here we will look at hermitian matrices. A **hermitian matrix** is one satisfying

$$\mathbf{M} = \mathbf{M}^\dagger \equiv (\mathbf{M}^T)^* \quad (\text{hermitian}) . \quad (6)$$

This just means that the components of a hermitian matrix satisfy $M_{ij} = M_{ji}^*$.

We say that the vector v_n is an **eigenvector** of the matrix \mathbf{M} if it satisfies

$$\mathbf{M}v_n = \lambda_n v_n , \quad (7)$$

where λ_n is a number called an **eigenvalue** of \mathbf{M} . If \mathbf{M} is hermitian, the eigenvalues λ_n are all real, and the eigenvectors may be taken to be orthonormal:

$$v_m^\dagger v_n = \delta_{nm} . \quad (8)$$

So we can take the v_n to be our basis vectors, and write an arbitrary vector A in this basis as

$$A = \sum_n A_n v_n . \quad (9)$$

where the A_n are in general complex numbers. This is a convenient choice if we wish to know what is the action of the hermitian matrix \mathbf{M} when it multiplies the vector A :

$$\mathbf{M}A = \sum_n A_n \mathbf{M}v_n = \sum_n A_n \lambda_n v_n . \quad (10)$$

2 Dirac notation for vectors

Now let us introduce Dirac notation for vectors. We simply rewrite all the equations in the above section in terms of bras and kets. We replace

$$V \rightarrow |V\rangle , \quad V^\dagger \rightarrow \langle V| , \quad A^\dagger B \rightarrow \langle A|B\rangle . \quad (11)$$

Suppose we have basis vector $|i\rangle$, analogous to the \hat{e}_i , which form a complete orthonormal set:

$$\begin{aligned} \langle i|j\rangle &= \delta_{ij} && (\text{orthonormality}) \\ \sum_i |i\rangle\langle i| &= \mathbf{1} && (\text{completeness}) , \end{aligned} \quad (12)$$

where $\mathbf{1}$ is the **identity operator**; it has the property $\mathbf{1}|\psi\rangle = |\psi\rangle$ for any $|\psi\rangle$.

Then any vector $|V\rangle$ may be expanded in this basis as

$$|V\rangle = \mathbf{1}|V\rangle = \sum_i |i\rangle\langle i|V\rangle \equiv \sum_i V_i |i\rangle , \quad V_i \equiv \langle i|V\rangle . \quad (13)$$

Note that $\langle V|i\rangle = V_i^*$.

As before, we can use the eigenvectors of a hermitian operator for our basis vectors. Matrices become **operators** in this language, $\mathbf{M} \rightarrow \hat{M}$. Then the eigenvalue equation becomes

$$\hat{M}|n\rangle = \lambda_n|n\rangle, \quad (14)$$

where the λ_n are real and we can take the $|n\rangle$ kets to be orthonormal: $\langle m|n\rangle = \delta_{mn}$. Then we can write

$$\hat{M}|V\rangle = \hat{M} \sum_n V_n|n\rangle = \sum_n V_n \hat{M}|n\rangle = \sum_n V_n \lambda_n|n\rangle. \quad (15)$$

3 Dirac notation for quantum mechanics

Functions can be considered to be vectors in an infinite dimensional space, provided that they are normalizable. In quantum mechanics, wave functions can be thought of as vectors in this space. We will denote a quantum state as $|\psi\rangle$. This state is **normalized** if we make it have unit norm: $\langle\psi|\psi\rangle = 1$.

Measurable quantities, such as position, momentum, energy, angular momentum, spin, etc are all associated with operators which can act on $|\psi\rangle$. If \hat{O} is an operator corresponding to some measurable quantity, its **expectation value** is given by $\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle$. Note that since

$$\langle A|\hat{O}|B\rangle^* = \langle B|\hat{O}^\dagger|A\rangle,$$

(*check this in the case of finite length vectors and matrices!*) it follows that if your measurable quantity is real (and they always are!) then $\langle\hat{O}\rangle = \langle\hat{O}\rangle^*$ implies that

$$\langle\psi|\hat{O}|\psi\rangle = \langle\psi|\hat{O}^\dagger|\psi\rangle,$$

or that $\hat{O} = \hat{O}^\dagger$.

Conclusion: Measurable quantities are associated with hermitian operators.

In order to compute expectation values for given quantum states, it is often useful to choose a convenient basis. I will discuss three common bases that are often used: the position eigenstate basis, the momentum eigenstate basis, and the energy eigenstate basis.

3.1 Position eigenstate basis: $|x\rangle$

The position operator $\hat{x} = \hat{x}^\dagger$ is a hermitian operator, and we can use its eigenvectors as an orthonormal basis. The state $|x\rangle$ is defined to be the eigenstate of \hat{x} with eigenvalue x :

$$\hat{x}|x\rangle = x|x\rangle. \quad (16)$$

What is new here is that the eigenvalues x are not discrete, and so we use the Dirac δ -function for normalization:

$$\langle x|x'\rangle = \delta(x - x') \quad (\text{orthonormality}). \quad (17)$$

The states $|x\rangle$ form a complete basis for our space and

$$\int dx |x\rangle\langle x| = \hat{1} \quad (\text{completeness}) \quad (18)$$

Note that the sum over discrete basis vectors in eq. (12) has been replaced by an integral. Also, the unit operator $\hat{1}$ has replaced the unit matrix \mathbf{I} . Therefore we can expand our state $|\psi\rangle$ in terms of the $|x\rangle$ basis vectors:

$$|\psi\rangle = \hat{1} |\psi\rangle = \int dx |x\rangle\langle x|\psi\rangle = \int dx \psi(x)|x\rangle, \quad (19)$$

where we have defined $\psi(x) \equiv \langle x|\psi\rangle$. This $\psi(x)$ is nothing but our familiar wavefunction. In the present language, $\psi(x)$ are the *coordinates* of the our state $|\psi\rangle$ in the $|x\rangle$ basis.

Note that in eq. (19) we inserted the unit operator in the guise of a integral over $|x\rangle\langle x|$ — this technique is very powerful, and is called **“inserting a complete set of states”**.

If we have normalized $|\psi\rangle$ so that $\langle\psi|\psi\rangle = 1$, it follows that

$$1 = \langle\psi|\psi\rangle = \langle\psi|\hat{1}|\psi\rangle = \int dx \langle\psi|x\rangle\langle x|\psi\rangle = \int dx \psi^*(x)\psi(x). \quad (20)$$

This is the usual normalization condition we have seen.

Computing $\langle\hat{x}^n\rangle$ for our state is particularly easy in the $|x\rangle$ basis, since $|x\rangle$ is an eigenstate of the operator \hat{x}^n :

$$\begin{aligned} \langle\hat{x}^n\rangle &= \langle\psi|\hat{x}^n|\psi\rangle \\ &= \int dx \langle\psi|\hat{x}^n|x\rangle\langle x|\psi\rangle \\ &= \int dx x^n \langle\psi|x\rangle\langle x|\psi\rangle \\ &= \int dx x^n \psi^*(x)\psi(x). \end{aligned} \quad (21)$$

In the next section I will discuss measuring $\langle\hat{p}\rangle$, using the position eigenstate basis.

3.2 Momentum eigenstate basis: $|p\rangle$

Another useful basis is formed by the eigenstates of the momentum operator \hat{p} :

$$\hat{p}|p\rangle = p|p\rangle, \quad \langle p|p'\rangle = \delta(p-p'), \quad \int dp |p\rangle\langle p| = \hat{1}. \quad (22)$$

We can expand $|\psi\rangle$ in the momentum basis as

$$|\psi\rangle = \int dp |p\rangle\langle p|\psi\rangle = \int dp \phi(p)|p\rangle, \quad \phi(p) \equiv \langle p|\psi\rangle. \quad (23)$$

We see that $\phi(p)$ is just the wavefunction in the momentum basis. As in the above section, we can easily compute expectation values such as $\langle\hat{p}^n\rangle$ using this basis.

It is interesting to ask how we can translate between the $|x\rangle$ and the $|p\rangle$ bases. For this, we need to know the quantity $\langle x|p\rangle$. We can get this by knowing that $\psi(x)$ and $\phi(p)$ are Fourier transforms of each other:

$$\psi(x) = \int \frac{dp}{\sqrt{2\pi\hbar}} \phi(p) e^{ipx/\hbar} . \quad (24)$$

We can rewrite this as

$$\psi(x) = \langle x|\psi\rangle = \int \frac{dp}{\sqrt{2\pi\hbar}} \langle p|\psi\rangle e^{ipx/\hbar} . \quad (25)$$

Inserting a complete set of states on the left hand side of the above equation we get

$$\int dp \langle x|p\rangle \langle p|\psi\rangle = \int \frac{dp}{\sqrt{2\pi\hbar}} \langle p|\psi\rangle e^{ipx/\hbar} , \quad (26)$$

implying that

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} . \quad (27)$$

Using this result we can also compute (here $|y\rangle$ is an eigenvector of \hat{x} with eigenvalue y):

$$\begin{aligned} \langle y|\hat{p}|x\rangle &= \int dp \langle y|\hat{p}|p\rangle \langle p|x\rangle \\ &= \int dp p \langle y|p\rangle \langle p|x\rangle \\ &= \int dp \frac{p}{2\pi\hbar} e^{ip(y-x)/\hbar} \\ &= i \frac{\partial}{\partial x} \int \frac{dp}{2\pi} e^{ip(y-x)/\hbar} \\ &= i\hbar \frac{\partial}{\partial x} \delta(x-y) . \end{aligned} \quad (28)$$

Therefore if we know $\psi(x)$ but not $\phi(p)$, we can still compute $\langle \hat{p} \rangle$ as

$$\begin{aligned} \langle \hat{p} \rangle = \langle \psi|\hat{p}|\psi\rangle &= \int dy \int dx \langle \psi|y\rangle \langle y|\hat{p}|x\rangle \langle x|\psi\rangle \\ &= \int dy \int dx \psi^*(y) \left(i\hbar \frac{\partial}{\partial x} \delta(x-y) \right) \psi(x) . \end{aligned} \quad (29)$$

Integrating by parts with respect to x (ignoring the boundary terms at $x = \pm\infty$, which vanish) we get

$$\begin{aligned} \langle \hat{p} \rangle &= \int dy \int dx \psi^*(y) \delta(x-y) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x) \\ &= \int dx \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x) \end{aligned} \quad (30)$$

So we see that in the x representation, $\hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$.

3.3 Energy eigenstates: $|n\rangle$

Finally, another operator of interest is the Hamiltonian \hat{H} which gives the energy. Up to now, the Hamiltonians we have seen take the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) . \quad (31)$$

The time dependent Schrodinger equation can be written as

$$i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = \hat{H} |\psi, t\rangle . \quad (32)$$

You can think of $|\psi, t\rangle$ as a vector moving around in our vector space as a function of time, and the above equation governs how it moves.

Since \hat{p} and \hat{x} are hermitian, then \hat{H} is also hermitian, provided that the potential $V(x)$ is a real function. Therefore we can use eigenstates $|n\rangle$ of \hat{H} as basis vectors:

$$\hat{H}|n\rangle = E_n|n\rangle , \quad \langle m|n\rangle = \delta_{mn} , \quad \sum_n |n\rangle\langle n| = \hat{1} . \quad (33)$$

Note that this eigenvalue equation is simply the time-independent Schrödinger equation, and that since \hat{H} is hermitian, the eigenvalues E_n are real numbers. (Here I have assumed that the energy eigenvalues E_n are discrete; this is correct for bound states but not scattering states. For states with continuous eigenvalue, replace the δ_{mn} by $\delta(m - n)$, and the \sum_n by $\int dn$.)

Then we can expand $|\psi, t\rangle$ in this basis, with time-dependent coefficients:

$$|\psi, t\rangle = \sum_n c_n(t) |n\rangle . \quad (34)$$

Plugging this into the Schrödinger equation eq. (32) we find

$$i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = \sum_n i\hbar \frac{dc_n(t)}{dt} |n\rangle = \sum_n \hat{H} c_n(t) |n\rangle = \sum_n E_n c_n(t) |n\rangle \quad (35)$$

Since the $|n\rangle$ form an orthonormal basis, it is easy to show that the above equation implies

$$i\hbar \frac{dc_n(t)}{dt} = E_n c_n(t) \implies c_n(t) = e^{-iE_n t/\hbar} c_n(0) . \quad (36)$$

Therefore the solution for $|\psi, t\rangle$ is

$$|\psi, t\rangle = \sum_n e^{-iE_n t/\hbar} c_n(0) |n\rangle . \quad (37)$$

So all we need to know is what are $c_n(0)$ (the initial conditions at $t = 0$), and the solutions $|n\rangle$, E_n to the time-independent Schrödinger equation, eq. (33). Note that

$$\langle \psi, t | = \sum_n e^{iE_n t/\hbar} c_n(0)^* \langle n | . \quad (38)$$

If $|\psi, t\rangle$ is normalized, it follows that

$$1 = \langle \psi, t | \psi, t \rangle = \sum_m \sum_n c_m^*(t) c_n(t) \langle m | n \rangle = \sum_n |c_n(t)|^2 = \sum_n |c_n(0)|^2 . \quad (39)$$

Note that in the coordinate basis, where $\hat{x} \rightarrow x$, $\hat{p} \rightarrow -i\hbar d/dx$.

$$\langle x | n \rangle = u_n(x) , \quad (40)$$

where

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] u_n(x) = E_n u_n(x) . \quad (41)$$

Solving this sort of equation for different potentials $V(x)$ (and generalizations in 3 dimensions) what we will be doing for the rest of this quarter.

3.4 Comments

Why are these bases we have discussed necessarily different from each other? For example, can't we find a basis in which both \hat{p} and \hat{x} are simple? No. If we had a state $|x, p\rangle$ which was simultaneously an eigenstate of \hat{x} (with eigenvalue x) and \hat{p} (with eigenvalue p) it would follow that

$$\begin{aligned} [\hat{x}, \hat{p}] |x, p\rangle &= \hat{x}\hat{p}|x, p\rangle - \hat{p}\hat{x}|x, p\rangle \\ &= p\hat{x}|x, p\rangle - x\hat{p}|x, p\rangle \\ &= (px - xp)|x, p\rangle = 0 \end{aligned} \quad (42)$$

since x and p are ordinary numbers, and commute both with each other and with operators \hat{p} and \hat{x} . But we know that

$$[\hat{x}, \hat{p}] = i\hbar \hat{1} \quad (43)$$

(we don't normally write the $\hat{1}$) which is inconsistent with the previous result, and so there cannot be such a state as $|x, p\rangle$.

The result is that a state $|\psi\rangle$ cannot simultaneously be an eigenstate of two operators that do not commute.

For the hydrogen atom, we will find that we can find basis states which are simultaneously eigenstates of \hat{H} , $\hat{\mathbf{L}} \cdot \hat{\mathbf{L}}$, and \hat{L}_z , where \mathbf{L} refers to the angular momentum vector. We will discuss a normalized basis of angular momentum states later in the course.