SUPPLEMENTARY NOTES ON DIRAC NOTATION, QUANTUM STATES, ETC.

These notes were prepared by Prof. Jaffe for the 8.05 course which he taught in 1996. In next couple of weeks we will cover all of this material in lecture, though not in as much detail. I am handing them out early so you have an additional source for the material that you can read as we go along, perhaps also filling in some gaps.

There are three main parts.

1. The "Postulates of Quantum Mechanics".
2. Completeness and orthonormality.
3. An extended example of the use of Dirac notation — position and momentum.

Note that Prof. Jaffe had not yet introduced spin as a two state system at the time he distributed these notes. I recommend that as you read these notes, at every step of the way you think how to apply them to the two state system.

If you are having difficulty with the concepts we have covered in the first part of 8.05 please study these notes carefully. The notes are written using Dirac Notation throughout. One of the purposes is to give you lots of exposure to this notation.

If, after reading these notes, it all still seems confusing, or overly formal, give yourself time. We will study some simple physical examples (especially the harmonic oscillator and the "two state systems" which we have already introduced) where you will learn by doing.

Here, then, are Prof. Jaffe's notes:

1 The Postulates of Quantum Mechanics

I'm not a lover of "postulates". In general it is better to develop the ideas gradually and let them sink in and become familiar, rather than to announce a set of postulates and try to derive physics from them. In this case, however, we began 8.05 with a wide range of backgrounds, so it is worthwhile to make sure we have a common understanding of how quantum mechanics works in general. Hence this section.

1.1 First Postulate

At each instant the state of a physical system is represented by a **ket** $|\psi\rangle$ *in the space of states.*

Comments

- The space of states is a vector space. This postulate is already radical because it implies that the *superposition* of two states is again a state of the system. If $|\psi_1\rangle$ and $|\psi_2\rangle$ are possible states of a system, then so is

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle, \tag{1}$$

  where a_1 and a_2 are complex numbers. Imagine that $|\psi_1\rangle$ is a particle with one value for some property like location and $|\psi_2\rangle$ is the same particle with a different value. In quantum mechanics we must allow ourselves to consider which superpose a particle in different locations. We were forced to do this by the results of experiments like the double-slit diffraction of electrons.

- The space of states comes equipped with the concept of an *inner product* which we abstract from wave mechanics. The inner product associates a complex number to any two states

$$(|\psi\rangle, |\phi\rangle) \equiv \langle\psi|\phi\rangle = \int dx \psi^*(x)\phi(x). \tag{2}$$

  Here we have used two different notations. The first defines the inner product as an operation acting on two states in the ket space. The second introduces another copy of the space of states called the "bra space", and defines the inner product as an operation involving one element of the bra space and one element of the ket space. Either way, the inner product reduces to the integral overlap of the two states when evaluated in terms of wavefunctions — $\int \psi^*\phi$. From (2) we see that

$$\langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle. \tag{3}$$

1.2 Second Postulate

Every observable attribute of a physical system is described by an operator that acts on the kets that describe the system.

Comments

- By *convention*, an operator $\hat{\mathcal{A}}$ acting on a ket $|\psi\rangle$ is denoted by left multiplication,

$$\hat{\mathcal{A}} : |\psi\rangle \to |\psi'\rangle = \hat{\mathcal{A}}|\psi\rangle. \tag{4}$$

You are used to this concept in the context of wave-mechanics, where the concept of a *state* is replaced by that of a *wavefunction*. A system (a particle in a potential, for example) is described by a wavefunction $\psi(x)$ in wave-mechanics. Some simple observable attributes of such a system are its *position*, its *momentum* and its *energy*. These are represented in wave mechanics by *differential operators*, $\hat{X} = x$, $\hat{P} = -i\hbar\frac{d}{dx}$ and $\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ respectively. These operators act on a wavefunction by left-multiplication, like

$$\hat{P}\psi(x) = -i\hbar\frac{d\psi}{dx} \tag{5}$$

- It is important to recognize that acting with an operator on a state in general changes the state. Again think back to wave mechanics. The lowest energy eigenfunction in a square well ($0 \leq x \leq L$) is

$$\psi(x) = \sqrt{2/L}\sin\pi x/L \quad \text{for} \quad 0 \leq x \leq L. \tag{6}$$

When we act on this wavefunction with $\hat{P}$, for example, we get

$$\hat{P}\psi(x) = -i\hbar\pi/L\sqrt{2/L}\cos\pi x/L \tag{7}$$

which is no longer an energy eigenfunction at all. So the operator changed the state of the particle.

- For every operator, there are special states that are not changed (except for being multiplied by a constant) by the action of an operator,

$$\hat{\mathcal{A}}|\psi_a\rangle = a|\psi_a\rangle. \tag{8}$$

These are the *eigenstates* and the numbers a are the *eigenvalues* of the operator. You have encountered them in wave mechanics, now they show up in the abstract space of states.

1.3 Third Postulate

The only possible result of the measurement of an observable $\mathcal{A}$ is one of the eigenvalues of the corresponding operator $\hat{\mathcal{A}}$.

Comments

- This is, of course, the origin of the word "quantum" in quantum mechanics. If the observable has a continuous spectrum of eigenvalues, like the position x or the momentum p, then the statement is not surprising. If it has a discrete spectrum, like the Hamiltonian for an electron bound to a proton (the hydrogen atom), then the statement is shocking. A measurement of the energy of the hydrogen atom will yield

only one of a discrete set of values. Needless to say, this postulate reflects mountains of experimental evidence such as the discrete *spectral lines* observed in the radiation from a tube of hot hydrogen gas.

- Since we measure only real numbers, the eigenvalues of operators corresponding to observables had better be real. Operators with real eigenvalues are *hermitian*.

  The eigenstates of a hermitian operator have some important properties.

  - They are orthogonal

$$\langle a_j|a_k\rangle \equiv (a_j, a_k) = \int dx \psi^*_{a_j}(x)\psi_{a_k}(x) = \delta_{jk}. \tag{9}$$

  - They span the space of states, so they form a *basis*. This means than an arbitrary state can be expanded as a sum (with complex coefficients) of the eigenstates of a hermitian operator. For this reason we say that the set of states is "complete".

1.4 Fourth Postulate

When a measurement of an observable $\mathcal{A}$ is made on a generic state $|\psi\rangle$, the probability of obtaining an eigenvalue a_n is given by the square of the inner product of $|\psi\rangle$ with the eigenstate $|a_n\rangle$, $|\langle a_n|\psi\rangle|^2$.

Comments

- The states are assumed to be normalized. Usually we normalize our states to unity,

$$\begin{aligned} \langle\psi|\psi\rangle &= 1 \\ \langle a_j|a_k\rangle &= \delta_{jk}. \end{aligned} \tag{10}$$

  Sometimes this is not possible. The case of momentum eigenstates, $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp ipx/\hbar$, is the classic example. In this case we must use "δ-function" or "continuum" normalization as discussed in Section 2.

- The complex number, $\langle a_n|\psi\rangle$ is known as the "probability amplitude" or "amplitude", for short, to measure a_n as the value for $\mathcal{A}$ in the state $|\psi\rangle$.

- Here is the algebraic exercise suggested by this postulate. First, any state can be expanded as a superposition of $\mathcal{A}$-eigenstates (see Post. 3),

$$|\psi\rangle = \sum_n c_n |a_n\rangle. \tag{11}$$

Next use the orthonormality of the $\mathcal{A}$ eigenstates to find an expression for the expansion coefficients c_n,

$$\begin{aligned} \langle a_j|\psi\rangle &= \sum_n c_n \langle a_j|a_n\rangle \\ &= c_j. \end{aligned} \tag{12}$$

So,

$$|\psi\rangle = \sum_n \langle a_n|\psi\rangle \cdot |a_n\rangle. \tag{13}$$

The $\cdot$ is added just to make clear the separation between the complex number $\langle a_n|\psi\rangle$ and the state $|a_n\rangle$. So, the component of $|\psi\rangle$ along the "direction" of the n^{th} eigenstate of $\mathcal{A}$ is given by $\langle a_n|\psi\rangle$. The measurement operation yields the result a_n with a probability proportional to the square of this component, $|\langle a_n|\psi\rangle|^2$.

- The probability of obtaining *some result* is unity. For states normalized to unity,

$$|\langle\psi|\psi\rangle|^2 = \sum_m \sum_n c_m^* c_n \langle a_m|a_n\rangle. \tag{14}$$

Using $|\langle\psi|\psi\rangle| = 1$ and $\langle a_m|a_n\rangle = \delta_{mn}$, we get

$$\sum_n |c_n|^2 = 1 \tag{15}$$

- According to the usual rules of probability, we can compute the "expected value" of the observable $\mathcal{A}$. If the probability to observe a_n is $|c_n|^2$ then the expected value (denoted $\langle\mathcal{A}\rangle$) is

$$\langle\mathcal{A}\rangle = \sum_n a_n |c_n|^2. \tag{16}$$

- When there is more than one eigenstate with the same eigenvalue, then this discussion needs a little bit of refinement. We'll let this go until we need to confront it.

1.5 Fifth Postulate

Immediately after the measurement of an observable $\mathcal{A}$ has yielded a value a_n, the state of the system is the normalized eigenstate $|a_n\rangle$.

Comments

- Known picturesquely as the "collapse of the wavepacket", this is the most controversial of the postulates of quantum mechanics, and the most difficult to get comfortable with. It is motivated by experience with repeated measurements. If an experimental sample is prepared in a state $|\psi\rangle$ then it is observed that a measurement of $\mathcal{A}$ can

yield a variety of results a_n with probabilities $|\langle a_n|\psi\rangle|^2$. Identically prepared systems can yield different experimental outcomes. This is encompassed by the fourth postulate. However, if $\mathcal{A}$ is measured with outcome a_n on a given system, and then is immediately *remeasured*, the results of the second measurement *are not statistically distributed,* the result is always a_n again. Hence this postulate.

- The collapse of the wavepacket preserves the normalization of the state. If $|\psi\rangle$ and $|a_n\rangle$ are both normalized to unity, then the measurement process replaces $|\psi\rangle$ by $|a_n\rangle$, *not by* $|\langle a_n|\psi\rangle|^2 \cdot |a_n\rangle$.

1.6 Sixth Postulate

The time evolution of a quantum system preserves the normalization of the associated ket. The time evolution of the state of a quantum system is described by $|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$, *for some unitary operator* $\hat{U}$.

Comments

- We have not got to this subject yet. I include it for completeness.
- Under time evolution, a state $|\psi\rangle$ moves through the space of states on a trajectory we can define as $|\psi(t)\rangle$. The preservation of the norm of the state is associated with conservation of probability. If the observable A is energy, for example, then the statement (15) says that the probability to find the system with *some value for the energy* is unity when summed over all possible values. For this to remain true as time goes on, it is necessary for the norm of the state to stay unity.
- Soon we will show that this postulate requires $|\psi\rangle$ to obey a differential equation of the form
$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle \tag{17}$$
where $\mathcal{H}$ is a hermitian operator (we know it as the Hamiltonian). This is Schroedinger's equation written as an operator equation in the space of states (as opposed to a differential equation in the space of wavefunction).

2 Bases and Operators

In this section I want to go over two topics not treated in sufficient detail in lecture. First, more about orthonormality and completeness, and second, some of the properties of hermitian operators.

2.1 Orthonormality and Completeness

We are working in the space of states $\mathcal{S}$ of a quantum system. The states are denoted by kets, $|\psi\rangle$, or equivalently by bras $\langle\psi|$. We will assume from the start that it is possible to find a basis for this space. The process for finding a basis is discussed in courses in linear algebra. Simply put, one chooses a state, and includes it in the basis. Next one chooses another. If it is proportional to the first, one discards it. If not, one puts it in the basis. On to another. If it is a linear combination of the first two, it is not "new" and is discarded. If it is not a linear combination of the first two, it must be added to the basis. This continues until one has the largest possible set of linearly independent states, which is the basis.

We will have to deal with two different types of bases:

- Denumerable

  Denumerable $\equiv$ *countable*, meaning the states can be put into one-to-one correspondence with the integers. We can denote them by $\{|n\rangle\}$, where $n = 1, 2, 3, \ldots$ The energy eigenstates of the one-dimensional harmonic oscillator are a good example.

- Non-denumerable

  Here the elements of the basis cannot be counted. Instead they are denoted $|z\rangle$, labelled by a continuous variable, z, that ranges from $-\infty < z < \infty$. The eigenstates of position and momentum are the classic examples.

Of course there are other cases, where the basis requires two integer labels, or two continuous labels, or one of each. These are handled by simple generalizations of the analysis given here.

Our space of states has an inner product, $\langle\psi|\phi\rangle$. Using the inner product it is always possible to generate an *orthonormal* basis from one originally possessing no special properties with respect to the inner product. The process of making a basis orthonormal is called the "Schmidt orthogonalization process". It is explained in courses on linear algebra. I am going to skip it because we will see that the eigenstates of hermitian operators are automatically orthogonal. All we need to do to make them into an orthonormal basis is to divide out their length: $|\psi\rangle \to \sqrt{\langle\psi|\psi\rangle}|\psi\rangle$, so $\langle\psi|\psi\rangle = 1$.

I need to say how "orthonormality" is defined. If we were dealing with a finite dimensional vector space (like Euclidean 3-space), then orthonormality means that the inner product of two different basis elements is zero and the inner product of a basis vector with itself is unity: $\vec{v}_j \cdot \vec{v}_k = \delta_{jk}$. This generalizes directly to the case of a *denumerable basis*

$$\langle m|n\rangle = \delta_{mn} \tag{18}$$

but not to a non-denumerable basis. The symbol $\delta_{zz'}$ doesn't make sense — how closely equal do z and z' have to be before δ takes on the value 1? For a *non-denumerable* basis, we *postulate* an orthonormality relation more suited to continuous variables,

$$\langle z|z'\rangle = \delta(z - z') \tag{19}$$

where $\delta(z)$ is Dirac's δ-function. This is known as "continuum normalization". My hope is that you'll accept this as a candidate for an orthonormality condition and pursue its consequences with me.

Anyone who has studied Fourier Series and Fourier Integrals will recognize these two different orthonormality conditions. The independent *sine* functions, $\sqrt{\frac{2}{L}}\sin n\pi x/L$, that enter into Fourier Series satisfy an orthonormality condition like (18), where the inner product is defined as the integral from 0 to L. On the other hand, the independent functions that appear in Fourier Integrals, $\frac{1}{\sqrt{2\pi}}\exp iqx$, obey an orthonormality condition with a δ-function like (19).

There is a fancy way to state orthonormality that is very useful in quantum mechanics. First let's develop it in the case of denumerable bases. Take an arbitrary ket and expand it in the orthonormal basis $\{|n\rangle\}$,

$$|\psi\rangle = \sum_n c_n|n\rangle. \tag{20}$$

Using the orthonormality of the basis states we obtain an equation for the expansion coefficients,

$$c_n = \langle n|\psi\rangle, \tag{21}$$

and substitute back into (20), to obtain

$$|\psi\rangle = \sum_n \langle n|\psi\rangle \cdot |n\rangle. \tag{22}$$

The "dot" is again added to the equation explicitly to remind us that each term in the sum is the product of a complex number (*c-number*) $\langle a|\psi\rangle$ and a ket $|\psi\rangle$.

Now we do some Dirac trickery, by rearranging the terms in (22) and separating them in a suggestive manner,

$$\begin{aligned} |\psi\rangle &= \sum_n |n\rangle \cdot \langle n|\psi\rangle \\ &= \left[\sum_n |n\rangle\langle n|\right] \quad |\psi\rangle. \end{aligned} \tag{23}$$

In the last version the quantity in square-brackets plays the role of *the identity operator*,

$$1 = \sum_n |n\rangle\langle n| \tag{24}$$

Acting on the state $|\psi\rangle$, it gives $|\psi\rangle$ back again. Also it is placed properly (acting by left multiplication) for an operator in the ket space.

Perhaps it will help to make the analogy to ordinary vectors in 3-space. Expanding an arbitrary vector in a Cartesian basis (call the basis vectors $\hat{e}_j$, $j = 1, 2, 3$ and keep track

of transposes) we get

$$\begin{aligned}\vec{v} &= \sum_j (\hat{e}_j^T \cdot \vec{v}) \;\; \hat{e}_j \\ &= \left[\sum_j \hat{e}_j \hat{e}_j^T\right] \;\cdot\; \vec{v}. \end{aligned} \tag{25}$$

So the quantity $\sum_j \hat{e}_j \hat{e}_j^T$ seems to play the role of the identity. Well, if we write

$$\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \hat{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \hat{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{26}$$

and explicitly construct the 3×3 matrix $\sum_j \hat{e}_j \hat{e}_j^T$, it is easy to see it is the *unit matrix*. Our result, (24) is the extension of this result to a denumerably infinite dimensional space.

Finally I want to generalize (24) to non-denumerable bases. Since the label for the basis states is continuous, *we must integrate over it* in the analog of (20)

$$|\psi\rangle = \int_{-\infty}^{\infty} dz c(z) |z\rangle. \tag{27}$$

Note that the *function* $c(z)$ has taken the place of the expansion coefficients c_n. To find the analog of (21), we take the inner product with $\langle z'|$,

$$\langle z'|\psi\rangle = \int_{-\infty}^{\infty} dz c(z) \langle z'|z\rangle, \tag{28}$$

use $\langle z'|z\rangle = \delta(z - z')$ and perform the integral over z, leaving

$$c(z) = \langle z|\psi\rangle \tag{29}$$

just like (21). Now substitute back into (27) and rearrange the terms as we did in the denumerable case,

$$|\psi\rangle = \left[\int_{-\infty}^{\infty} dz |z\rangle\langle z|\right] |\psi\rangle \tag{30}$$

from which we extract

$$1 = \int_{-\infty}^{\infty} dz |z\rangle\langle z| \tag{31}$$

2.2 Operators and Hermitian Conjugation

Here I want to derive some of the properties of hermitian operators. First, however, lets review the derivation of hermitian conjugation.

2.2.1 Hermitian Conjugation

If $\hat{\mathcal{A}}$ is an operator defined by its action on the kets,

$$\hat{\mathcal{A}} : |\psi\rangle \rightarrow |\psi'\rangle = \hat{\mathcal{A}}|\psi\rangle, \tag{32}$$

then the hermitian conjugate of $\hat{\mathcal{A}}$, denoted $\hat{\mathcal{A}}^\dagger$, is defined to be the operator that has the same action on the bras,

$$\hat{\mathcal{A}}^\dagger : \langle\psi| \rightarrow \langle\psi'| = \langle\psi|\hat{\mathcal{A}}^\dagger, \tag{33}$$

The quantity $\hat{\mathcal{A}}|\psi\rangle$ is again a state in $\mathcal{S}$. To emphasize that fact we could put it into a ket notation,

$$\hat{\mathcal{A}}|\psi\rangle = |\hat{\mathcal{A}}\psi\rangle \tag{34}$$

The equivalent statement for the bra space is

$$\langle\psi|\hat{\mathcal{A}}^\dagger = \langle\hat{\mathcal{A}}\psi| = \langle\psi'|. \tag{35}$$

Note that we *do not* denote the bra by $\langle\hat{\mathcal{A}}^\dagger\psi|$, because it is the state with the same attributes as $|\psi'\rangle = |\hat{\mathcal{A}}\psi\rangle$.

Consider the inner product of $|\psi'\rangle$ defined in (32) with some arbitrary state $|\phi\rangle$

$$\langle\phi|\psi'\rangle \equiv \langle\phi|\hat{\mathcal{A}}|\psi\rangle \tag{36}$$

This defines a new kind of expression, with an operator sandwiched between a bra and a ket. Think of it as follows: when $\hat{\mathcal{A}}$ operates on $|\psi\rangle$, it creates some ket which one can overlap with $|\phi\rangle$. Completely equivalently, one can view $\hat{\mathcal{A}}$ as an operator on the bra space, tranforming the bra $\langle\phi|$ to a new element of the bra space, $\langle\phi|\hat{\mathcal{A}}$, which then overlaps with $|\psi\rangle$. The notation defined in (36) with $\hat{\mathcal{A}}$ between bra and ket includes both points of view and is the one we'll generally use.

Quantities of the form $\langle\phi|\hat{\mathcal{A}}|\psi\rangle$ are called "matrix elements". They are *c-numbers* and measure the capacity of the operator $\hat{\mathcal{A}}$ to provide overlap between the two states.

Complex conjugation of matrix elements involves hermitian conjugation of operators. Consider

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle^* = \langle\phi|\psi'\rangle^* \tag{37}$$

Using the complex conjugation property of the inner product, $\langle\phi|\psi'\rangle^* = \langle\psi'|\phi\rangle$, and (35) we find

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle^* = \langle\psi|\hat{\mathcal{A}}^\dagger|\phi\rangle \tag{38}$$

If the operator $\hat{\mathcal{A}}$ is hermitian, then its matrix elements have a simple behavior: complex conjugation is equivalent to exchanging the bra and the ket.

2.2.2 Eigenvalues and eigenstates of a hermitian operator

Here we show that the eigenvalues of a hermitian operator are real and that the eigenstates of a hermitian operator form an orthonormal set. Let's define the eigenkets and eigenvalues of some operator $\hat{\mathcal{A}}$ in the usual fashion

$$\hat{\mathcal{A}}|a_k\rangle = a_k|a_k\rangle \tag{39}$$

To be definite, we have assumed the eigenvalues are countable, and we've labelled the states by their eigenvalues.

From the definition of $\hat{\mathcal{A}}^\dagger$ we see that $\langle a_k|$ is an eigenbra of $\hat{\mathcal{A}}^\dagger$ with eigenvalue a_k^*,

$$\langle a_k|\hat{\mathcal{A}}^\dagger = a_k^*\langle a_k| \tag{40}$$

Let us restrict ourselves to hermitian operators, $\hat{\mathcal{A}}^\dagger = \hat{\mathcal{A}}$. Then take the inner product of (39) with the state $|a_k\rangle$ to obtain,

$$\langle a_k|\hat{\mathcal{A}}|a_k\rangle = a_k\langle a_k|a_k\rangle. \tag{41}$$

If $\hat{\mathcal{A}}$ is hermitian, then the matrix element $\langle a_k|\hat{\mathcal{A}}|a_k\rangle$ is real, as is the norm $\langle a_k|a_k\rangle$. So if we take the complex conjugate of (41) we conclude that *the eigenvalues of a hermitian operator are real*.

Next take the inner product of (39) with an eigenstate belonging to a different eigenvalue of $\hat{\mathcal{A}}$, say a_j,

$$\langle a_j|\hat{\mathcal{A}}|a_k\rangle = a_k\langle a_j|a_k\rangle. \tag{42}$$

Next write the eigenvalue equation for the eigenbra $\langle a_j|$,

$$\langle a_j|\hat{\mathcal{A}} = a_j\langle a_j|, \tag{43}$$

where we used both that $\hat{\mathcal{A}}$ is hermitian, and that a_j is real. Finally take the inner product of (43) with the eigenket $|a_k\rangle$,

$$\langle a_j|\hat{\mathcal{A}}|a_k\rangle = a_j\langle a_j|a_k\rangle. \tag{44}$$

If we compare (42) with (44) (subtract the two equations), we see that

$$\langle a_j|a_k\rangle = 0 \quad \text{if} \quad a_j \neq a_k. \tag{45}$$

So the eigenstates belonging to different eigenvalues of a hermitian operator are necessarily orthogonal. Next, choose the norm of the eigenstates to be unity and we have an orthonormal set of eigenstates for every hermitian operator.

There is one lacuna in this derivation. If two eigenstates share the same eigenvalue (the eigenvalue is said to be *degenerate*), we have not shown that the eigenstates are orthogonal. The flaw is fairly simple to repair: it is always possible to choose linear combinations of the

set of states belonging to the same eigenvalue so that they are orthogonal to one another, and of course any linear combination is still orthogonal to the eigenstates corresponding to different eigenvalues.

It is more difficult to show that the set of orthonormal eigenvectors of a hermitian operator is complete. It mirrors the completeness proof for Fourier Series or Fourier Integrals, which you may have encountered in other courses. Accepting completeness, we see that hermitian operators generate complete orthonormal bases for our space of states.

2.2.3 Operators as matrices in an orthonormal basis

The objects of interest in quantum mechanics are matrix elements of the form

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle. \tag{46}$$

If we make use of an orthonormal basis we can reduce the manipulation of matrix elements to matrix algebra. We consider denumerable and non-denumerable bases in turn.

Suppose the space of states has a denumerable basis, $\{|n\rangle\}$. We may expand both $|\psi\rangle$ and $|\phi\rangle$ in this basis,

$$\begin{aligned} |\psi\rangle &= \sum_n \langle n|\psi\rangle \cdot |n\rangle \\ |\phi\rangle &= \sum_m \langle m|\phi\rangle \cdot |m\rangle \end{aligned} \tag{47}$$

and substitute in (46).

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle = \sum_n \sum_m \langle\phi|m\rangle \cdot \langle m|\hat{\mathcal{A}}|n\rangle \cdot \langle n|\psi\rangle \tag{48}$$

a double sum over products of three complex numbers. To make (48) simpler in appearance, we define

$$\begin{aligned} \psi_n &\equiv \langle n|\psi\rangle \\ \phi_m &\equiv \langle m|\phi\rangle \\ A_{mn} &\equiv \langle m|\hat{\mathcal{A}}|n\rangle \end{aligned} \tag{49}$$

so (48) now reads

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle = \sum_m \sum_n \phi_m^* A_{mn} \psi_n \tag{50}$$

or

$$\langle\phi|\hat{\mathcal{A}}|\psi\rangle = \phi^\dagger A \psi \tag{51}$$

where A is the matrix of complex numbers whose mn^{th} component is A_{mn}, ψ is the column vector whose n^{th} component is ψ_n, and $\phi^\dagger$ is the row vector whose m^{th} component is ϕ_m^*. This is the origin of the term "Matrix Mechanics" that was originally applied to this

formulation of quantum mechanics. States are represented by vectors and operators by matrices.

Now consider the case of a non-denumerable basis $|z\rangle$. We start with (46). The expansions given in (47) are replaced by integrals

$$\begin{aligned} |\psi\rangle &= \int_{-\infty}^{\infty} dz \langle z|\psi\rangle \cdot |z\rangle \\ |\phi\rangle &= \int_{-\infty}^{\infty} dz \langle z|\phi\rangle \cdot |z\rangle. \end{aligned} \tag{52}$$

The *c-number* $\langle z|\psi\rangle$ is a *function* of the parameter z, so we denote it

$$\langle z|\psi\rangle = \psi(z). \tag{53}$$

When we substitute these decompositions of the states into (46) we will encounter a matrix element of the form $\langle z|\hat{\mathcal{A}}|z'\rangle$, which is a *c-number* function of the the two variables z and z', so we denote it,

$$\langle z|\hat{\mathcal{A}}|z'\rangle = A(z, z'). \tag{54}$$

Putting this all together in the case of a non-denumerable basis we obtain,

$$\langle \phi|\hat{\mathcal{A}}|\psi\rangle = \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \phi^*(z) A(z, z') \psi(z') \tag{55}$$

Vectors generalize to functions, matrices generalize to functions of two variables, and matrix multiplication generalizes to integration. We still talk about the states as vectors and the operators as "matrix elements" even in the case of non-denumerable bases. Next we'll go through the example of position and momentum eigenstates in an attempt to put all this together.

3 Position and Momentum in Dirac Notation

We are now ready to apply all this formalism to some physically interesting cases. The simplest, and most important, place to start is with the operators that dominate wave mechanics: position, x, and momentum p. [For simplicity we consider only one space dimension, the generalization to three dimensions is obvious.]

On the basis of everyday experience with the mechanics of classical systems, we *assume* the existence of two observables, position and momentum. We assume that measurement of position or momentum yield values from the continuum of real numbers.[1] Given the discussion of the previous two sections, we can assume the existence of

[1]Note: we could be wrong! Sometimes the quantum world is fundamentally unlike the classical one. There are cases where, for example, the momentum of a quantum particle is quantized. But until we encounter a disagreement with experiment, we will follow the natural path.

- Two hermitian operators, $\hat{X}$ and $\hat{P}$
- Two complete, orthonormal sets of eigenkets, $|x\rangle$, and $|p\rangle$, obeying

$$\begin{aligned} \hat{X}|x\rangle &= x|x\rangle \\ \hat{P}|p\rangle &= p|p\rangle \\ \langle x|y\rangle &= \delta(x-y) \\ \langle p|q\rangle &= \delta(p-q) \end{aligned} \tag{56}$$

  with x and p both real.

Notice that the existence of the eigenstates, and the reality of the eigenvalues follow from the postulates of quantum mechanics. The orthonormality condition is the one we choose for non-denumerable bases.

So far, we have not given any information defining a relation between x and p. We would have written down the same statements about two coordinates, x_1 and x_2, for example. The standard thing to do to connect x and p would be to postulate the *commutator* between X_{op} and P_{op}, but the reason for postulating $[\hat{X}, \hat{P}] = i\hbar$ won't be clear until we talk about "Canonical Quantization" in a few weeks. Instead I propose we rely on our knowledge of wave mechanics to tell us the *position space wavefunction for a momentum eigenstate*, namely,

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}, \tag{57}$$

which embodies the observation that momentum eigenstates propagate like plane waves.

First let's check the normalization of (57). This will give us an opportunity to use the completeness relation for non-denumerable states. We demand $\langle q|p\rangle = \delta(q-p)$. We want to convert this to an expression in terms of coordindate space wavefunctions, so we insert a complete set of coordinate eigenstates,

$$\begin{aligned} \langle q|p\rangle &= \langle q|1|p\rangle \\ &= \int_{-\infty}^{\infty} dx \langle q|x\rangle \cdot \langle x|p\rangle \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx e^{i(p-q)x/\hbar} \\ &= \delta(q-p) \end{aligned} \tag{58}$$

where the last step uses the Fourier representation for the δ-function (see the Appendix of Gasiorowicz).

Next let's look a coordinate space wavefunctions and the way the position and momentum operators are represented in coordinate space. An arbitrary state $|\psi\rangle$ can be expressed as a superposition of coordinate eigenstates,

$$|\psi\rangle = \int_{-\infty}^{\infty} dx |x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \langle x|\psi\rangle \cdot |x\rangle = \int_{-\infty}^{\infty} dx \psi(x)|x\rangle, \tag{59}$$

where we have defined $\langle x|\psi\rangle = \psi(x)$. Note this is the *standard* definition of the coordinate space wavefunction of the that $|\psi\rangle$, since $\langle x|\psi\rangle$ is the amplitude to find the state $|\psi\rangle$ at the position x.

How does $\hat{X}$ act on $|\psi\rangle$? Using (59) and working slowly step by step we easily find

$$\begin{aligned}
\hat{X}|\psi\rangle &= \hat{X}\int_{-\infty}^{\infty} dy\,|y\rangle\langle y|\psi\rangle \\
&= \int_{-\infty}^{\infty} dy\hat{X}|y\rangle\langle y|\psi\rangle \\
&= \int_{-\infty}^{\infty} dy\,y\,|y\rangle\langle y|\psi\rangle \\
&= \int_{-\infty}^{\infty} dy\,y\,\psi(y)|y\rangle\ . \qquad (60)
\end{aligned}$$

So,

$$\langle x|\hat{X}|\psi\rangle = \int_{-\infty}^{\infty} dy\,\psi(y)\,\langle x|y\rangle = \int_{-\infty}^{\infty} dy\,\psi(y)\,\delta(x-y) = x\,\psi(x)\ , \qquad (61)$$

and we recover the familiar fact that when $\hat{X}$ acts on the state $|\psi\rangle$ whose coordinate space wave function is $\psi(x)$ the resulting state has coordinate space wave function is $x\,\psi(x)$.

How does $\hat{P}$ act on $|\psi\rangle$? To answer this, let's find the coordinate space wavefunction of the state $|\Psi\rangle \equiv \hat{P}|\psi\rangle$. As a first step, we look at a momentum eigenstate,

$$\begin{aligned}
\langle x|\hat{P}|p\rangle &= p\langle x|p\rangle \\
&= p\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \\
&= -i\hbar\frac{d}{dx}\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \\
&= -i\hbar\frac{d}{dx}\langle x|p\rangle. \qquad (62)
\end{aligned}$$

So the coordinate space wave function of the state $\hat{P}|\psi\rangle$ is $-i\hbar$ times the derivative of the wavefunction of $|\psi\rangle$. Now let's look at an arbitrary state. Define $|\Psi\rangle \equiv \hat{P}|\psi\rangle$. Then,

$$\begin{aligned}
\langle x|\Psi\rangle &= \langle x|\hat{P}|\psi\rangle \\
&= \int_{-\infty}^{\infty} dp\langle x|\hat{P}|p\rangle\cdot\langle p|\psi\rangle \\
&= \int_{-\infty}^{\infty} dp(-i\hbar\frac{d}{dx}\langle x|p\rangle)\cdot\langle p|\psi\rangle \\
&= -i\hbar\frac{d}{dx}\langle x|\left[\int_{-\infty}^{\infty} dp|p\rangle\langle p|\right]|\psi\rangle \\
&= -i\hbar\frac{d}{dx}\psi(x), \qquad (63)
\end{aligned}$$

where we have liberally used the completeness relation for momentum eigenstates, $\int dp|p\rangle\langle p| = 1$. So we conclude

$$\hat{P}|\psi\rangle = |\Psi\rangle \Rightarrow \Psi(x) = -i\hbar\frac{d\psi}{dx}, \tag{64}$$

a standard result from wavemechanics. So we say that the "coordinate space representation of the momentum operator" is $-i\hbar\frac{d}{dx}$. If you want an exercise to check your understanding, try to show that the momentum space representation of the position operator is $i\hbar\frac{d}{dp}$.

Finally let's look at the coordinate space matrix elements of the position and momentum operators, $\langle x|\hat{X}|y\rangle$ and $\langle x|\hat{P}|y\rangle$. The first is easy,

$$\begin{aligned}\langle x|\hat{X}|y\rangle &= y\langle x|y\rangle \\ &= y\delta(x-y).\end{aligned} \tag{65}$$

$\hat{X}$ is a "local" operator in position space; it connects states only if they have the same eigenvalue. This is the continuum analog of a diagonal matrix: if we view $\langle x|\hat{X}|y\rangle \equiv f(x,y)$ as a matrix, only the diagonal ($x = y$) elements are non-zero.

The momentum operator is a little harder. Start with $\langle x|\hat{P}|\psi\rangle$ from (63)

$$\langle x|\hat{P}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x) \tag{66}$$

and insert a complete set of position eigenstates after $\hat{P}$,

$$\begin{aligned}\langle x|\hat{P}|\psi\rangle &= \langle x|\hat{P}\int_{-\infty}^{\infty} dy|y\rangle\langle y|\psi\rangle \\ &= \int_{-\infty}^{\infty} dy\langle x|\hat{P}|y\rangle\cdot\langle y|\psi\rangle \\ &= \int_{-\infty}^{\infty} dy\langle x|\hat{P}|y\rangle\psi(y).\end{aligned} \tag{67}$$

Comparing (66) and (67) we conclude

$$\langle x|\hat{P}|y\rangle = -i\hbar\delta(x-y)\frac{d}{dy}, \tag{68}$$

which you can check by substitution. So the momentum operator is almost, but not quite, local in coordinate space. The derivative shows that acting with $\hat{P}$ involves two infinitesmally nearby points in coordinate space.

Just as an arbitrary matrix is not diagonal, so an arbitrary operator matrix element in coordinate space is not local. If $\hat{\mathcal{T}}$ is some unspecified operator, then acting on an arbitrary state $|\psi\rangle$, we find,

$$\begin{aligned}\langle x|\hat{\mathcal{T}}|\psi\rangle &\equiv \psi_{\mathcal{T}}(x) \\ &= \int_{-\infty}^{\infty} dy\langle x|\hat{\mathcal{T}}|y\rangle\cdot\langle y|\psi\rangle \\ \psi_{\mathcal{T}}(x) &= \int_{-\infty}^{\infty} dy\ T(x,y)\ \psi(y).\end{aligned} \tag{69}$$

So the operator $\hat{\mathcal{T}}$ gets represented by its coordinate space matrix elements $T(x,y) = \langle x|\hat{\mathcal{T}}|y\rangle$, which acts as an *integral transform* on the wavefunction $\psi(x)$. Only when $\hat{\mathcal{T}}$ is local (like $\hat{X}$) or nearly local (like $\hat{P}$) does the integral go away leaving a simpler situation.