PHY 115A
Lecture Notes 3:
Formalism
(Griffith's Chapter 3)

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Chapter 3

Formalism

3.1 Matter Waves

Early in the development of quantum mechanics it became clear that light was quantized as photons with discrete energy:

$$E = h\nu$$

but for a massless particle, we know that:

$$E = pc$$

and:

$$pc = h\nu$$

so that:

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

where λ is the wavelength of the light. De Broglie made the hypothesis that matter was also described by a wave with frequency:

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

and wavelength:

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

We are using the reduced Planck's constant:

$$\hbar = \frac{h}{2\pi}$$

so we write these relations equivalently as:

$$E = h\nu = \hbar(2\pi\nu) = \hbar\omega$$

and:

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k$$

Recall that in general a right traveling wave has the format:

$$f(k\,x - \omega\,t)$$

for $k > 0$ and $\omega > 0$. So we can imagine several different functional forms for de Broglie's "matter waves" traveling left:

$$\Psi_1(x, t) = \cos(kx - \omega t)$$

or:

$$\Psi_2(x, t) = \sin(kx - \omega t)$$

or

$$\Psi_3(x, t) = \exp(ikx - i\omega t)$$

where we don't care about the amplitude of the function yet. But take care to note that:

$$g(-k\,x + \omega\,t) = g(-(k\,x - \omega\,t))$$

is also a right traveling wave, because it can be written as:

$$f(k\,x - \omega\,t) \equiv g(-(k\,x - \omega\,t))$$

But since:

$$\cos(-k\,x + \omega\,t) = \cos(k\,x - \omega\,t)$$

we don't need to consider that case. And since:

$$\sin(-k\,x + \omega\,t) = -\sin(k\,x - \omega\,t)$$

and we don't care about the amplitude of the function yet, we can ignore that as well. That only leaves one additional possibility to consider:

$$\Psi_4(x, t) = \exp(-ikx + i\omega t)$$

It seems like we could use any of these four options, but let's see what happens when we try to construct a standing wave by adding an equal mixture of right traveling and left traveling waves. To switch to a left traveling wave, we just put:

$$k \to -k$$

Our standing wave using Ψ_1 is:

$$\Psi(x) = \cos(k\,x - \omega\,t) + \cos(-k\,x - \omega\,t)$$

but using:

$$\cos(\alpha + \beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$$

we conclude:

$$\Psi(x) = 2\cos(k\,x)\cos(\omega\,t)$$

which is an utter catastrophe, since the wave function vanishes everywhere whenever:

$$\omega t = \frac{n\pi}{2} \qquad\qquad n = 1, 3, 5$$

This would describe a particle that disappears and reappears from existence... not the theory we are trying to build! So we discard option Ψ_1. Likewise for Ψ_2:

$$\Psi(x) = \sin(k\,x - \omega\,t) + \sin(-k\,x - \omega\,t)$$

but using:
$$\sin(\alpha + \beta) = \sin(\alpha)\cos(\beta) + \cos(\alpha)\sin(\beta)$$

we conclude:
$$\Psi(x) = -2\cos(k\,x)\sin(\omega\,t)$$

which is another catastrophe, since the wave function vanishes everywhere whenever:
$$\omega t = n\pi \qquad\qquad n = 1, 2, 3, 4, 5$$

But there is no such problem with Ψ_3 where:

$$\Psi(x) = \exp(ik\,x - i\omega\,t) + \exp(-ik\,x - i\omega\,t) = 2\cos(kx)e^{-i\omega t}$$

this vanishes at specific locations in space, where the particle will never be found, but this is exactly what we would expect for a standing wave. The only time-dependent factor

$$e^{-i\omega t}$$

is never zero at any point in time. Similarly, for Ψ_4:

$$\Psi(x) = \exp(-ik\,x + i\omega\,t) + \exp(ik\,x + i\omega\,t) = 2\cos(kx)e^{i\omega t}$$

So it seems at this point that both Ψ_3 and Ψ_4 are valid options for a right-traveling matter waves, but if they are both valid, then we should be able to superimpose them:

$$\Psi_3(x, t) + \Psi_4(x, t) = \exp(ik\,x - i\omega\,t) + \exp(-ik\,x + i\omega\,t) = 2\cos(k\,x - \omega\,t)$$

which we already saw was a problematic right traveling wave. So we conclude that we can have Ψ_3 or Ψ_4, but **not both**. We choose the one that has $k > 0$ for a right traveling wave, so that our right traveling matter wave is finally uniquely identified as:

$$\Psi_{\mathrm{k}}(x, t) \equiv \exp(ik\,x - i\omega\,t) \tag{3.1}$$

with where:
$$p = \hbar k, \qquad \text{and} \qquad E = \hbar\omega.$$

For the free particle, we also have:
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{3.2}$$

and so:
$$\omega(k) = \frac{\hbar k^2}{2m} \tag{3.3}$$

The free particles have phase velocity:

$$v_{\mathrm{phase}} = \frac{\omega}{k} = \frac{\hbar k}{2m}$$

and group velocity:

$$v_{\mathrm{group}} = \frac{d\omega}{dk} = \frac{\hbar k}{m}$$

which is the classical velocity of the particle. In chapter 2, we showed that this phase velocity is the velocity of a wave packet consisting of waves with wave numbers close to k.

3.2   From Matter Waves to the Schrödinger Equation

With the matter waves in hand, we now will try to identify the wave equation that predicts matter waves for a free particle $(V(x) = 0)$, in the hope that we can generalize that equation in other contexts $(V(x) \neq 0)$.

The first thing we will try to do is determine the momentum of the matter wave. Now, knowing that:

$$\Psi_k(x, t) = \exp(ik\,x - i\omega\,t)$$

we can of course simply read off the wave number k and determine the momentum $p = \hbar k$. But we cannot *generalize* that approach to other wave functions $\Psi(x, t)$. In the general case, we will only know $\Psi(x, t)$, so we can only do things involving x and t. Here's something:

$$-i\hbar \frac{\partial}{\partial x} \Psi_k(x, t) = (-i\hbar)(ik)\Psi_k(x, t) = \hbar k \Psi_k(x, t) = p\Psi_k(x, t)$$

so we define the momentum operator:

$$\hat{p} \equiv -i\hbar \frac{\partial}{\partial x} \tag{3.4}$$

and note that for our matter wave for free particles:

$$\hat{p}\,\Psi_k(x, t) = p\,\Psi_k(x, t) \tag{3.5}$$

We say that the free particle solutions $\Psi_k(x, t)$ is an eigenstate of the momentum operator $\hat{p}$. Note that this is true only for eigenstates. For a general state with wave function $\Psi(x, t)$ generally:

$$\hat{p}\,\Psi(x, t) \neq p\,\Psi(x, t)$$

Note also that $\hat{p}$ and p are two very different things. Whereas p is just a number, $\hat{p}$ is a complicated beast: an operator that when given a wave function returns a (possibly different) wave function.

What about the position operator $\hat{x}$? Since we have access to x and t, for any wave function $\Psi(x, t)$, we need only write:

$$\hat{x} = x \tag{3.6}$$

and so for *any wave function $\Psi(x, t)$*

$$\hat{x}\,\Psi(x, t) = x\,\Psi(x, t)$$

which looks like any $\Psi(x, t)$ is also an eigenstate of $\hat{x}$, but that is not so, because x is not just a number here, and

$$x\,\Psi(x, t)$$

is a new wave function that is distinct from $\Psi(x, t)$.

Next we will try to find a recipe for determining the energy $E = \hbar\omega$ only through $\Psi(x, t)$. We can try something similar:

$$i\hbar \frac{\partial}{\partial t}\,\Psi_k(x, t) = (i\hbar)(-i\omega)\,\Psi_k(x, t) = \hbar\omega\,\Psi_k(x, t) = E\,\Psi_k(x, t)$$

We also know that for the free particle:

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

So let's find an operator $\hat{H}$ such that:

$$\hat{H}\Psi_k(x,t) = \frac{p^2}{2m}\Psi_k(x,t)$$

for our free particles. Working with our definition of the momentum operator:

$$\hat{H}\ \Psi_k(x,t) = \frac{p^2}{2m}\Psi_k(x,t) = \frac{p}{2m}(p\ \Psi_k(x,t)) = \frac{p}{2m}\left(-i\hbar\frac{\partial}{\partial x}\ \Psi_k(x,t)\right)$$

but p here is just a number (unlike $\hat{p}$ or $\partial/\partial x$) so we are free to move it right up against $\Psi_k(x,t)$ and continue on:

$$\hat{H}\ \Psi_k(x,t) = \frac{-i\hbar}{2m}\frac{\partial}{\partial x}(p\ \Psi_k(x,t)) = \frac{-i\hbar}{2m}\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\ \Psi_k(x,t)\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_k(x,t)$$

from which we read off the operator $\hat{H}$ for the free particle:

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

this is the Hamiltonian operator (for the free particle) which does not have any potential energy. For a general potential, we need to find an operator $\hat{V}$ and the total energy will be obtained by:

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

But the potentials we will encounter will depend only on x and t, so the operator $\hat{V}$ is trivial:

$$\hat{V} = V(\hat{x},t) = V(x,t)$$

So for the free particle with $V(x,t) = 0$ we have shown that:

$$i\hbar\frac{\partial}{\partial t}\Psi_k(x,t) = \hat{H}\ \Psi_k(x,t)$$

but our assumption is that when $V(x,t) \neq 0$ we can determine the possible states as solutions to the equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\ \Psi(x,t) \tag{3.7}$$

or equivalently

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\ \Psi(x,t) + V(x,t)\Psi(x,t) \tag{3.8}$$

So we have plausibly deduced the Schrödinger Equation from the deBroglie hypothesis via the Matter Waves.

3.3   Hilbert Space

In quantum mechanics, the state of a system is represented by a wave function, $\Psi(x,t)$ and we interpret $|\Psi(x,t)|^2$ as the probability density for measuring the particle at position x at time t. For this interpretation to work, we must have:

$$\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = 1$$

But for a function $f(x)$ to be a candidate for a wave function we need only statisfy the weaker condition:

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx = C < \infty$$

for then we can always just multiple $f(x)$ by $\sqrt{1/C}$ to obtain a properly normalized wave function. We call such a function a square-integrable function.

We saw in the Fourier Series appendix that periodic functions satisfy the axiomatic properties of an abstract vector space. What about square-integrable functions? They are closed under addition as a consequence of the Schwarz inequality:

$$\left| \int_a^b f(x)^* g(x)\, dx \right| \leq \sqrt{\int_a^b |f(x)|^2\, dx \int_a^b |g(x)|^2\, dx} \tag{3.9}$$

with which you should be able to show that if $f(x)$ and $g(x)$ are square integrable, then:

$$\int_{-\infty}^{+\infty} f(x) + g(x)\, dx < \infty$$

The other properties are of an abstract vector space are easy to establish for square integrable functions, as they follow immediately from the familiar algebraic properties of functions.

We define an inner product for this vector space as:

$$\langle f|g \rangle \equiv \int_a^b f(x)^* g(x)\, dx$$

Here again the Schwarz inequality shows that for vectors f and g the inner product is finite. Most of the properties of an inner product again follow directly from familiar algebraic properties. One subtlety arises when showing that:

$$\langle f|f \rangle = 0$$

if and only if:

$$f(x) = 0$$

To see the challenge, consider the (non-continuous) square-integrable function:

$$f(x) = \begin{cases} 1 & x = \pi \\ 0 & \text{otherwise} \end{cases}$$

which has $\langle f|f \rangle = 0$ but is not $f(x) = 0$. The solution is to define two functions f and g as equivalent (the same vector) whenever:

$$\int_{-\infty}^{+\infty} |f(x) - g(x)|^2\, dx = 0$$

So now clearly if:

$$\langle f|f \rangle = 0$$

then:

$$\int_{-\infty}^{+\infty} |f(x)|^2\, dx = 0$$

and so too:

$$\int_{-\infty}^{+\infty} |f(x) - 0|^2\, dx = 0$$

so that $f(x)$ is equivalent to $g(x) = 0$.

Last we turn to the property of completeness: any sequence of functions that gets closer and closer together will converge to a vector in the inner-product space. That is, if a sequence of functions $\{f_n(x)\}$ has the property that:

$$\int_{-\infty}^{+\infty} |f_n(x) - f_m(x)|^2 \, dx \to 0, \qquad \text{as} \qquad m, n \to \infty$$

then:

$$f_n(x) \to f(x), \qquad \text{as} \qquad n \to \infty$$

for some vector $f(x)$ in the vector space.

And with this property, we run into serious trouble, for we already know that $\delta(x)$ is the limit of a sequence of taller and narrower square-integrable functions, but it isn't itself square integrable. Nonetheless, the fact is that one can build a complete inner product space that contains the δ-function and the limits of any sequence of square-integrable functions. But to do so requires complicating **everything** in order to properly handle vectors like the δ function. Physicists make a different choice: we keep to our much simple definitions that apply perfectly well to the square integrable wave functions we encounter, and simply accept that we will also occasionally encounter the delta function posing as if it were an actual function. We find that, inevitably, we integrate this delta function away before obtaining any observable result.

The mathematical term for a complete inner-product space is a Hilbert Space. Apart from side-stepped the issue of completeness, we have shown that the square-integrable functions form a Hilbert Space. For the state described by wave function:

$$\Psi(x, t)$$

we will write this as a vector in Hilbert space like this:

$$|\Psi\rangle$$

.

3.4 Operators and Observables

An operator $\hat{O}$ in a Hilbert Space H is a mapping of vectors in H to vectors in H. We could just call it a function, but that terminology would be confusing as the vectors it has as input and output are themselves square-integrable functions. Given a vector $|\Psi\rangle$ in the Hilbert Space, an operator returns a (possibly new) vector $|\Phi\rangle$:

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

or we might choose to write that equivalently as:

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

where the LHS is an operator acting on the vector Ψ whereas the RHS is the vector obtained by acting on Ψ with the operator $\hat{O}$. We will only consider linear operators with the defining properties:

$$\hat{O}(|\Psi\rangle + |\Phi\rangle) = \hat{O} |\Psi\rangle + \hat{O} |\Phi\rangle$$

and:

$$\hat{O} (\alpha |\Psi\rangle) = \alpha \hat{O} |\Psi\rangle$$

We associate expectation values with inner products:

$$\langle O \rangle \equiv \langle \Psi | \hat{O} \Psi \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \, \hat{O} \, \Psi(x,t) \, dx$$

For an operator $\hat{O}$ we define its hermitian adjoint $\hat{O}^\dagger$ by the behavior:

$$\langle f | \hat{O}^\dagger g \rangle = \langle \hat{O} f | g \rangle$$

or equivalently:

$$\langle f | \hat{O} g \rangle = \langle \hat{O}^\dagger f | g \rangle$$

When an operator is its own hermitian adjoint:

$$\hat{Q}^\dagger = \hat{Q}$$

we call it a hermitian operator, and it's expectation value is real:

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q}^\dagger \Psi | \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle = \langle \Psi | \hat{Q} \Psi \rangle^* = \langle Q \rangle^*$$

Therefore, we associate physical observables with hermitian operators, as in "the observable $\hat{Q}$".

3.5   Determinate States

We've accepted that Quantum Mechanics is indeterminate, in the sense that if we prepare many copies of a system, each described by the same state vector $|\Psi\rangle$, and we repeat the same measurement for each copy, then the outcome of each of those measurements may be different.

Now we wish to consider if it is possible to prepare a system that is guaranteed to give a particular result q for the measurement of an observable $\hat{Q}$. We already know of one example of such a state: the stational solutions of the Schrodinger equations have definite energy, and we saw that they are Eigenenfunctions of the Hamiltonian operator. We can write this with our updated notation as:

$$\hat{H} | \Psi \rangle = E | \Psi \rangle$$

which says equivalently that they are Eigenvectors of the Hamilitonian operator. Let's see if this generalizes.

For a determinate state, every measurement results in q, so then:

$$\langle \hat{Q} \rangle = q$$

but also:

$$\sigma^2 = \langle \left(\hat{Q} - \langle Q \rangle \right)^2 \rangle = 0$$

and so:

$$0 = \langle \left(\hat{Q} - q \right)^2 \rangle = \langle \Psi | \left(\hat{Q} - q \right)^2 \Psi \rangle$$

but since $\hat{Q}$ is an observable and q is a real number $\hat{Q} - q$ is a hermitian operator so:

$$\langle \Psi | \left(\hat{Q} - q \right)^2 \Psi \rangle = \langle \left(\hat{Q} - q \right) \Psi | \left(\hat{Q} - q \right) \Psi \rangle = 0$$

but an axiomatic property of the inner product is that:

$$\langle f | f \rangle = 0 \iff | f \rangle = 0$$

so we have:

$$
\begin{aligned}
0 &= \left| \left(\hat{Q} - q \right) \Psi \right\rangle \\
0 &= \left(\hat{Q} - q \right) |\Psi\rangle \\
\hat{Q} |\Psi\rangle &= q |\Psi\rangle
\end{aligned}
$$

So, exactly as we found already for the specific case of the Hamiltonian operator, the eigenvectors of any observable (hermetian operator) $\hat{Q}$ are determinate states. Note that the vector 0 is never considered to be an eigenvector (as it would trivially be an eigenvector of every operator, adding nothing of value), but the value 0 can certainly be an eigenvalue.

3.6 Eigenvalues of Observables

Operators associated with physical observables, that is, hermitian operators, have a special property:

- **The eigenvalues of hermitian operators are real.** Suppose $|\Psi\rangle$ is an eigenvector of hermitian operator $\hat{Q}$ with eigenvalue q:

$$
\hat{Q} |\Psi\rangle = q |\Psi\rangle
$$

  We know that for a determinate state $\langle Q \rangle = q$, and since the expectation values of hermitian operators are real, then q is real too.

It's useful practice to work this result out explicitly:

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

so:

$$
\begin{aligned}
q \langle \Psi | \Psi \rangle &= q^* \langle \Psi | \Psi \rangle \\
(q - q^*) \langle \Psi | \Psi \rangle &= 0
\end{aligned}
$$

But by definition eigenvectors cannot be zero, so:

$$
|\Psi\rangle \neq 0 \implies \langle \Psi | \Psi \rangle \neq 0
$$

So

$$
q = q^*
$$

which shows that q is real.

The collection of eigenvalues of an operator is called its spectrum. In what follows we will consider discrete spectra and continuous spectra separately, but no matter the type of spectra **the eigenvalues of a hermitian operator are real.**

3.7 Eigenvectors of Observables with Discrete and Non-Degenerate Spectra

Let's consider the case of an operator $\hat{Q}$ with a discrete (whether finite or infinite) spectrum of eigenvalues $\{\alpha_i\}$. In this case, it is convenient to label the state vector of each determinate state by it's eigenvalue:

$$\hat{Q}\ket{\alpha_i} = \alpha_i \ket{\alpha_i}$$

If one vector is a scalar times another vector:

$$\ket{\alpha_i} = k\ket{\alpha_j}$$

we call them linearly dependent. When this is not the case they are linearly independent. Sometimes two linearly independent vectors $\ket{\alpha_i}$ and $\ket{\alpha_j}$ have the same eigenvalue for an operator $\hat{Q}$:

$$\alpha_i = \alpha_j$$

In this case, we call the spectrum degenerate. Here we are assuming the spectrum is non-degenerate, and tackle the minor complexity of degeneracy later.

In the case an operator with discrete non-generate spectrum, the determinate states have some useful properties:

- **They are orthogonal:**

$$
\begin{aligned}
\braket{\alpha_i | \hat{Q}\alpha_j} &= \braket{\hat{Q}\alpha_i | \alpha_j} \\
\alpha_j \braket{\alpha_i | \alpha_j} &= \alpha_i \braket{\alpha_i | \alpha_j} \\
(\alpha_j - \alpha_i) \braket{\alpha_i | \alpha_j} &= 0
\end{aligned}
$$

As we are assuming non-degenerate spectrum in this section:

$$\alpha_j \neq \alpha_i \implies \braket{\alpha_i | \alpha_j} = 0$$

Furthermore, as the $\ket{\alpha_i}$ are vectors in the Hilbert space of square-integrable functions, they can be properly normalized, so that:

$$\braket{\alpha_n | \alpha_m} = \delta_{nm}$$

.

- **They are complete.** Below we show this in the general case for a finite dimensional Hilbert space. We've also already seen it hold true in infinite dimensions in the case of the Fourier series solutions to the infinite square well potential. Beyond this, we will "assume the eigenfunctions of an observable are complete unless proven otherwise."

3.8 Generalized Statistical Interpretation

We've seen that the eigenvectors of an observable with a discrete non-degenerate spectrum have the "Big Three" properties: (1) they have real eigenvalues, (2) they be arranged to be orthonormal, and (3) they are complete. In this context, we are now ready to state **the most important material of this quarter**: the general statistical interpretation of the eigenfunctions of an observable.

Because of property (3), we can express any state vector $|\Psi\rangle$ as a sum of eigenvectors of **any** observable $\hat{Q}$:

$$|\Psi\rangle = \sum_n c_n(t) \, |\alpha_n\rangle \tag{3.10}$$

The sum over n here is over all possible values, which will vary from case to case (e.g. finite for bounds states of a square well, infinite starting at $n = 1$ for the infinite square well, infinite starting at 0 for the harmonic oscillator potential). The eigenvectors $|\alpha_n\rangle$ have the defining property:

$$\hat{Q} \, |\alpha_n\rangle = \alpha_n \, |\alpha_n\rangle$$

and property (1) informs us that every α_n is real.

Because of property (2), we can determine the coefficients $c_n(t)$ via Fourier's trick:

$$\langle \alpha_n | \Psi \rangle \;=\; \langle \alpha_n | \sum_m c_m(t) \alpha_m \rangle$$

Notice that we have changed the sum over n in Equation 3.10 to a sum over m. We can do this because it is a dummy variable (it has no meaning outside the sum), and we **must** do this in order to avoid getting confused the n in c_n. Moving out the sum and coefficient:

$$
\begin{aligned}
\langle \alpha_n | \Psi \rangle \;&=\; \sum_m c_m(t) \, \langle \alpha_n | \alpha_m \rangle \\
&=\; \sum_m c_m(t) \delta_{nm} \\
&=\; c_n(t)
\end{aligned}
$$

Memorize it if you must (even better to understand it well) but you will have to reproduce this entire calculation in some form on your final exam, and without resorting to any integrals!

Now let's see how to obtain the expectation value for the observable $\hat{Q}$:

$$
\begin{aligned}
\langle \hat{Q} \rangle \;&=\; \langle \Psi | \hat{Q} \Psi \rangle \\
&=\; \langle \sum_n c_n(t)\alpha_n | \hat{Q} \sum_m c_m(t)\alpha_m \rangle \\
&=\; \sum_{n,m} c_n^*(t) c_m(t) \, \langle \alpha_n | \hat{Q} \alpha_m \rangle \\
&=\; \sum_{n,m} c_n^*(t) c_m(t) \alpha_m \, \langle \alpha_n | \alpha_m \rangle \\
&=\; \sum_{n,m} c_n^*(t) c_m(t) \alpha_m \delta_{nm} \\
&=\; \sum_n |c_n(t)|^2 \, \alpha_n
\end{aligned}
$$

But our statistical intrepretation of an expectation value is the weighted average of possible outcomes, with the weight equal to the probability of each outcome. So evidently **the probability that a measurement will yield outcome α_n is $|c_n(t)|^2$.**

For this interpretation to work we should have:

$$\sum_n |c_n(t)|^2 = 1$$

and sure enough:

$$
\begin{aligned}
1 &= \langle \Psi | \Psi \rangle \\
&= \langle \sum_n c_n(t)\alpha_n | \sum_m c_m(t)\alpha_m \rangle \\
&= \sum_{n,m} c_n^*(t)c_m(t) \langle \alpha_n | \alpha_m \rangle \\
&= \sum_{n,m} c_n^*(t)c_m(t)\delta_{nm} \\
&= \sum_n |c_n(t)|^2
\end{aligned}
$$

To summarize: the eigenvectors of any observable $\hat{Q}$ have the defining property:

$$\hat{Q} |\alpha_n\rangle = \alpha_n |\alpha_n\rangle$$

These eigenvectors have the big three properties: (1) their eigenvalyes (α_n) are real, (2) they can be arranged to be orthonormal, and (3) they are complete. Therefore, any state vector can be expressed as a sum of eigenvectors:

$$|\Psi\rangle = \sum_n c_n(t) |\alpha_n\rangle$$

The probability that a measurement of the observable $\hat{Q}$ results in the particular real value α_n is $|c_n(t)|^2$.

Notice that as a logical consequence, the outcome of a measurement is limited to one of the eigenvalues of the operator. Furthermore, as we first discussed in Chapter 1 (but have done little with so far), the action of making a measurement causes the wave function to collapse. We can be more specific now, and say that after a measurement of outcome α_n, the wave function collapses [1] to the unique eigenstate corresponding to that eigenvalue (we are not considering degenerate spectra yet.)

$$|\Psi\rangle \longrightarrow |\alpha_n\rangle$$

So, assuming that the wave function does not evolve further, subsequence measurements of the observable $\hat{Q}$ will yield the value α_n with $|c_n(t)|^2 = 1 = 100\%$ certainty.

3.9   Eigenvectors of Hermitian Operators with Degenerate Spectra

If one vector is a scalar times another vector:

$$|\alpha_i\rangle = k |\alpha_j\rangle$$

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[1]There are other possible interpretations, but this is consistent with the Copenhagen interpretation which we will take as our baseline interpretation for this course.

we call them linearly dependent. When this is not the case they are linearly independent. Sometimes two linearly independent vectors $|\alpha_i\rangle$ and $|\alpha_j\rangle$ have the same eigenvalue for an operator $\hat{Q}$:

$$\alpha_i = \alpha_j$$

and in this case we say the spectrum is degenerate[2] In this case, even though we cannot assume these eigenfunctions are orthogonal, we can arrange them so. Consider the vector:

$$|x\rangle \equiv |\alpha_j\rangle - \langle\alpha_i|\alpha_j\rangle\,|\alpha_i\rangle$$

it is orthogonal to $|\alpha_i\rangle$ as we can see from:

$$\langle\alpha_i|x\rangle = \langle\alpha_i|\alpha_j\rangle - \langle\alpha_i|\alpha_j\rangle\,\langle\alpha_i|\alpha_i\rangle = 0$$

Furthermore, it cannot be zero for otherwise we would have:

$$|\alpha_j\rangle = \langle\alpha_i|\alpha_j\rangle\,|\alpha_i\rangle$$

and we already said $|\alpha_j\rangle$ and $|\alpha_i\rangle$ were linearly independent. Lastly, it too has eigenvalue α_j:

$$
\begin{aligned}
\hat{Q}\,|x\rangle &= \hat{Q}\,|\alpha_j\rangle - \langle\alpha_i|\alpha_j\rangle\,\hat{Q}\,|\alpha_i\rangle \\
&= \alpha_j\,|\alpha_j\rangle - \langle\alpha_i|\alpha_j\rangle\,\alpha_i\,|\alpha_i\rangle \\
&= \alpha_j\,|x\rangle
\end{aligned}
$$

This means $|x\rangle$ has the same eigenvalue as $|\alpha_j\rangle$ but is also orthogonal to $|\alpha_i\rangle$. So we need only normalize $|x\rangle$ and then redefine:

$$|\alpha_j\rangle \equiv |x\rangle$$

so that now:

$$\langle\alpha_i|\alpha_j\rangle = 0$$

even though:

$$\alpha_i = \alpha_j$$

We can extend this to any number of vectors with degenerate eigenvalues as needed to obtain an orthogonal set of eigenvectors. This process is called the Gram-Schmidt orthogonalization.

To summarize, for a degenerate discrete spectrum, the eigenvectors can be arranged, via the Gram-Schmidt orthogonalization, such that:

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$$

and thus arranged to have the same "Big Three" properties as do the eigenvectors of non-degenerate discrete spectrum.

As a consequence, the standard statistical interpretation applies for degenerate spectra in exactly the same manner as for non-degenerate spectra. The only minor subtlety is what happens in the case that the outcome of a measurement yields a degenerate result. In this case, the wave function still collapses, but now to a linear combination of the (degenerate) eigenvectors.

---

[2]By the way, be careful not to take our notation too literally here, we still have:

$$|\alpha_i\rangle \neq |\alpha_j\rangle$$

because it is completely clear which vector is which, even though $\alpha_i = \alpha_j$!

To illustrate, suppose the state vector is:

$$|\Psi\rangle = \frac{1}{2}\left(|\alpha_1\rangle + i\,|\alpha_2\rangle + \sqrt{2}\,|\alpha_3\rangle\right)$$

where $|\alpha_i\rangle$ are eigenfunctions of the observable $\hat{Q}$ and $\alpha_1 = \alpha_2$ but $\alpha_3 \neq \alpha_1$. The probability that a measurement of $\hat{Q}$ results in α_3 is:

$$\left|\frac{\sqrt{2}}{2}\right|^2 = \frac{1}{2}$$

After a measurement with outcome α_3 the wave function collapses to:

$$|\Psi\rangle \longrightarrow |\alpha_3\rangle$$

On the other hand, the probability that a measurement of $\hat{Q}$ results in $\alpha_1 = \alpha_2$ is:

$$\left|\frac{1}{2}\right|^2 + \left|\frac{i}{2}\right|^2 = \frac{1}{2}$$

After a measurement with outcome $\alpha_1 = \alpha_2$ the wave function collapses to:

$$|\Psi\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|\alpha_1\rangle + i\,|\alpha_2\rangle\right)$$

In all of the cases, we used our freedom to choose the overall phase of the wave-function, but notice that the relative phase of $|\alpha_1\rangle$ and $|\alpha_2\rangle$ is preserved by the collapse.

3.10   The Dirac Delta function and the Fourier Transform

It is both mathematically dubious and extremely useful to consider the Fourier Transform of the Dirac Delta function:

$$\widetilde{\delta}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x)e^{-ikx}dx = \frac{e^{-ik0}}{\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}}$$

and so we can write the Dirac delta function as:

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}dk \tag{3.11}$$

and by interchanging variables:

$$\delta(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}dx$$

As always when dealing with the Dirac delta function, these relations are only really valid within another integral, and that is precisely how we will use them in what follows.

By substitution of variables[3]

$$\delta(x - y) = \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ik(x-y)}dk$$

---

[3]Don't get confused here, we are still in one-dimension, and y is just a different dummy variable in the same direction as x. You can think of it as x' if you prefer, but x' doesn't show up well on the board, so we use y in lecture.

and:

$$\delta(k - l) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-l)x} dx$$

Equation 3.11 is a kind of shorthand for the Fourier Transform, for we can use to derive the Fourier and Inverse Fourier Transforms directly:

$$\begin{aligned}
\psi(x) &= \int_{-\infty}^{+\infty} \psi(y) \, \delta(x - y) \, dy \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi(y) \, e^{ik(x-y)} \, dk \, dy \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(y) \, e^{-iky} \, dy \right) dk
\end{aligned}$$

The quantity in parenthesis is just the fourier transform of $\psi(x)$, don't be fooled by the dummy variable y, so we have only to define:

$$\widetilde{\psi}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x) \, e^{-ikx} \, dx$$

and we have immediately:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \widetilde{\psi}(k) \, e^{ikx} \, dk$$

Notice we could have made other choices here about how to distribute the factor of $1/2\pi$, we've chosen to write these in the most symmetric fashion.

There's another very useful result that the delta function allows us to calculate relatively easily, the normalization of the Fourier transform:

$$\begin{aligned}
\int_{-\infty}^{+\infty} |\widetilde{\psi}(k)|^2 dk &= \int_{-\infty}^{+\infty} \widetilde{\psi^*}(k)\widetilde{\psi}(k) dk \\
&= \int_{-\infty}^{+\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx}\psi(x)dx \right)^* \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-iky}\psi(y)dy \right) dk \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi^*(x)\psi(y) \left(\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(x-y)}dk \right) dxdy \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi^*(x)\psi(y)\delta(x - y)dxdy \\
&= \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx
\end{aligned}$$

This is called Parseval's theorem.

3.11   Eigenvectors of Observables with Continuous Spectra

Let's consider the case of an operator $\hat{Q}$ with a continuous spectrum of eigenvalues $\{\alpha\}$. In this case, it is convenient to label the state vector of each determinate state by it's eigenvalue:

$$\hat{Q} \, |\alpha\rangle = \alpha \, |\alpha\rangle, \qquad \hat{Q} \, |\beta\rangle = \beta \, |\beta\rangle$$

where now there is no index i on the eigenvalues, as the spectrum is uncountably infinite. As $\hat{Q}$ is hermitian, the eigenvalues (α and β here) are real. Furthermore, we can show that:

$$\langle \alpha | \beta \rangle = 0, \qquad \text{for } \alpha \neq \beta$$

using the same calculation as for the discrete case, so the eigenfunctions are orthogonal too. As is our right as physicists, we may assume (until proven otherwise) that the eigenvectors are complete, so we can write:

$$|\Psi\rangle = \int_{-\infty}^{+\infty} a(\alpha) \, |\alpha\rangle \, d\alpha$$

where we have replaced the sum over discrete eigenvalues with an integral over continuous eigenvalues. We expect to be able to determine the coefficients $a(\beta)$ using Fourier's trick:

$$\langle \beta | \Psi \rangle \;\; = \;\; \int_{-\infty}^{+\infty} a(\alpha) \, \langle \beta | \alpha \rangle \, d\alpha$$

So for this to work, we need $\langle \beta | \alpha \rangle$ to pick out the particular value $a(\beta)$ from the integral. No ordinary function will do this, but the delta function. With:

$$\langle \beta | \alpha \rangle = \delta(\alpha - \beta)$$

we obtain:

$$\langle \beta | \Psi \rangle = a(\beta)$$

as expected.

Evidently, the eigenfunctions of continuous spectra are not normalizable! We therefore cannot have normal orthonormality, but we have instead what Griffith's calls "Dirac othonormality", which replaces the Kronecker delta with the Dirac delta function.

Let's look at some concrete examples:

- **Eigenvectors of the momentum operator:** For a concrete example, let's consider the eigenvectors of the momentum operator:

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

The state vector $|p\rangle$ has an associated wave function $\psi_p(x)$, for which the momentum operator takes it's familiar form $\hat{p} = -i\hbar d/dx$, so we have:

$$-i\hbar \frac{d}{dx} \psi_p(x) = p \psi_p(x)$$

with solutions:

$$\psi_p(x) = A e^{ipx/\hbar}$$

These are none other than our plane wave solutions to the free particle SE. This is no surprise, since the free-particle Hamiltonian depends only on $\hat{p}$, and so:

$$\hat{H} \, |p\rangle = \frac{\hat{p}^2}{2m} \, |p\rangle = \frac{p^2}{2m} \, |p\rangle$$

That is, eigenvectors of $\hat{p}$ are also eigenvectors of $\hat{H}$.

We can check the orthogonality by calculating the inner product of the $|p\rangle$ with another eigenvector of the momentum operator $|q\rangle$:

$$\langle q|p\rangle = |A|^2 \int_{-\infty}^{+\infty} e^{i(p-q)x/\hbar} dx = |A|^2 \, 2\pi\hbar \, \delta(p-q)$$

So if we take:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

Then:

$$\langle q|p\rangle = \delta(p-q)$$

which is Dirac orthonormality, exactly as we expect. We can write any state vector as an integral over the eigenvectors:

$$|\Psi\rangle = \int_{-\infty}^{+\infty} c(p) \, |p\rangle \, dp$$

and obtain the coefficients from Fourier's Trick:

$$
\begin{aligned}
\langle p|\Psi\rangle &= \int_{-\infty}^{+\infty} c(q) \, \langle p|q\rangle \, dq \\
&= \int_{-\infty}^{+\infty} c(q) \, \delta(q-p) \, dq \\
&= c(p)
\end{aligned}
$$

- **Eigenvectors of the position operator:** Next let's consider the eigenvectors $|y\rangle$ of the position operator:

$$\hat{x} \, |y\rangle = y \, |y\rangle$$

Here we are using y to indicate a specific value of the variable x. The state vector $|y\rangle$ has an associated wave function $\psi_y(x)$ for which:

$$\hat{x}\psi_y(x) = x\psi_y(x) = y\psi_y(x)$$

where x is a variable and y is a specific value. The solution is:

$$\psi_y(x) = A\delta(x-y)$$

for then:

$$x\psi_y(x) = xA\delta(x-y) = yA\delta(x-y) = y\psi_y(x)$$

as needed. We can check orthogonality:

$$\langle y|z\rangle = |A|^2 \int_{-\infty}^{+\infty} \delta(x-y)\delta(x-z)dx = |A|^2\delta(y-z)$$

If we choose $A = 1$ we have:

$$\langle y|x\rangle = \delta(x-y)$$

From completeness we have:

$$|\psi\rangle = \int_{-\infty}^{+\infty} c(x) \, |x\rangle \, dp$$

and Fourier's Trick gives the expected outcome:

$$
\begin{aligned}
\langle y|\psi\rangle &= \int_{-\infty}^{+\infty} c(x)\,\langle y|x\rangle\,dx \\
&= \int_{-\infty}^{+\infty} c(x)\delta(y-x)dx \\
&= c(x)
\end{aligned}
$$

and also:

$$
\langle y|\psi\rangle = \int_{-\infty}^{+\infty} \delta(x-y)\psi(x)dx = \psi(y)
$$

or equivalently:

$$
\psi(x) = \langle x|\psi\rangle
$$

which at last precisely connects our Hilbert space state vectors to the wave function: the wave function is the inner product of the position eigenvector with the state vector.

3.12   Position and Momentum Space Wave Functions

We found in the previous sections that the eigenvector $|y\rangle$ of position has wave function:

$$
\psi_y(x) = \delta(x-y)
$$

which led to the formal connection between the state vector and wave function:

$$
\langle x|\Psi\rangle = \Psi(x,t)
$$

The eigenvector of momentum $|p\rangle$ has wave function:

$$
\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}
$$

Now let's consider the inner product:

$$
\langle p|\Psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} \Psi(x,t)e^{-ipx/\hbar}dx
$$

which we see is just the Fourier Transform of $\Psi(x,t)$, but with $k \to p/\hbar$. We call this the momentum space wave function:

$$
\langle p|\Psi\rangle = \widetilde{\Psi}(p,t)
$$

We can expand the wave function as:

$$
|\Psi\rangle = \int c(x)\,|x\rangle\,dx
$$

or

$$
|\Psi\rangle = \int c(p)\,|p\rangle\,dp
$$

But we can determine the coefficients, as always, using Fourier's trick:

$$
c(x) = \langle x|\Psi\rangle = \Psi(x,t)
$$

and

$$c(p) = \langle p | \Psi \rangle = \widetilde{\Psi}(p, t)$$

So:

$$|\Psi\rangle = \int \Psi(x, t) |x\rangle \, dx$$

or

$$|\Psi\rangle = \int \widetilde{\Psi}(p, t) |p\rangle \, dp$$

In the case of discrete eigenvalues, we have:

$$|\Psi\rangle = \sum_n c_n |\alpha_n\rangle$$

and we saw that the probability of measuring value α_n was

$$P(n) = |c_n|^2 = |\langle \alpha_n | \Psi \rangle|^2$$

In the continuous case we have:

$$P(a \leq x \leq b) = \int_a^b |\Psi(x)|^2 dx = \int_a^b |\langle x | \Psi \rangle|^2 dx$$

and

$$P(a \leq p \leq b) = \int_a^b |\widetilde{\Psi}(p)|^2 dp = \int_a^b |\langle p | \Psi \rangle|^2 dp$$

3.13   Summary of Determinate States

The eigenfunctions of hermitian operators (observables) have the "Big Three" properties: (1) their eigenvalues of real, (2) they can be arranged into an orthonormal basis, and (3) they are complete. If the spectrum is degenerate, the Gram-Schmitt procedure must be used to produce an orthonormal basis. If the spectrum is continuous, the normal orthonormality is replaced by Dirac orthonormality.

Property	Discrete	Continuous
Orthonormality	$\langle \alpha_m | \alpha_n \rangle = \delta_{mn}$	$\langle \alpha | \beta \rangle = \delta(\alpha - \beta)$
Completeness	$|\Psi\rangle = \sum_n c_n |\alpha_n\rangle$	$|\Psi\rangle = \int_{-\infty}^{+\infty} c(\alpha) |\alpha\rangle$
Normalization	$\sum_n |c_n|^2 = 1$	$\int_{-\infty}^{+\infty} |c(\alpha)|^2 = 1$

3.14   The Generalized Uncertainty Principle

3.15   Commuting Observables

3.16   The Energy-Time Uncertainty Principle

3.17   Dirac Notation

In this course, we started with position-space wave functions $\Psi(x, t)$. We saw that the wave functions form a Hilbert space with an inner product:

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

More recently, we've come to associate the position-space wave function with a state vector:

$$|\Psi\rangle$$

with:

$$\Psi(x, t) = \langle x|\Psi(t)\rangle$$

That is, the value of the wave function at value x is the inner product of the state vector $|\Psi(t)\rangle$ with the eigenvectors of position $|x\rangle$. The state $|\Psi(t)\rangle$ is more general than the position-space wave function, because, e.g. the state of the system can be equally well expressed by a momentum-space wave function:

$$\widetilde{\Psi}(p, t) = \langle p|\Psi(t)\rangle$$

We are going to drop the explicit time dependence in what follows (because there is more than enough going on already) and write:

$$\Psi(x) = \langle x|\Psi\rangle$$

it follows that:

$$\Psi^*(x) = \langle \Psi|x\rangle$$

While $\Psi(x)$ and $\Psi^*(x)$ are connected via complex conjugation:

$$\Psi(x) \xleftrightarrow{\text{CC}} \Psi^*(x)$$

we should also have some connection (to be defined) between $|\Psi\rangle$ and $\langle\Psi|$:

$$|\Psi\rangle \xleftrightarrow{\text{dual}} \langle\Psi|$$

But what is $\langle\alpha|$? It's not an operator. An operator $\hat{O}$

$$\hat{O}\,|\Psi\rangle = |\Phi\rangle$$

acts on a vector to a new vector, so we can say it maps a vector to a vector. But:

$$(\langle\alpha|)\,|\beta\rangle = \langle\alpha|\beta\rangle \in \mathbb{C}$$

so $\langle\alpha|$ maps a vector to scalar. It's a complex function but takes a vector as input. Just as our position-space wave functions were part of a Hilbert space, the $\bar{\alpha}$ are elements of a dual space. But we don't really need to delve into those details, we need only recognize that when we the product of a

3.18 Optional: Completeness of Eigenvectors of a Hermitian Operator in Finite Dimensions

This is just for fun, don't worry about this material. Here we will show that the eigenvectors of a Hermitian operator Q are complete in any n dimensional Hilbert space.

It is evidently true for $n = 1$. We will assume it is true for $n - 1$ and show that it is true for n. The proof will follow from induction.

Take any normalized eigenvector of $\hat{Q}$ in an n-dimensional Hilbert space V can label it by it's eigenvalue λ_n:

$$\hat{Q} \ket{\lambda_n} = \lambda_n \ket{\lambda_n}$$

Now consider the subspace $S^\perp$ of all vectors perpendicular to $\ket{\lambda_n}$:

$$S^\perp \equiv \{\ket{x} \text{ such that } \braket{x|\lambda_n} = 0\}$$

The subspace $S^\perp$ has dimension $n - 1$ by construction. To see this, note that $S^\perp$ has dimension n at most, so we can write any $\ket{x}$ in $S^\perp$ in terms of n orthonormal basis vectors, including $\ket{\lambda_n}$

$$\ket{x} = A_n \ket{\lambda_n} + A_1 \ket{x_1} + A_2 \ket{x_2} + \ldots + A_{n-1} \ket{x_{n-1}}$$

but

$$A_n = \braket{\lambda_n|x} = 0$$

so really:

$$\ket{x} = A_1 \ket{x_1} + A_2 \ket{x_2} \ldots A_{n-1} \ket{x_{n-1}}$$

and we see that $S^\perp$ has $n - 1$ dimensions as intended.

Next we'll show that the $n - 1$ dimensional subspace $S^\perp$ is closed under $\hat{Q}$, so that we can consider $\hat{Q}$ as a Hermitian operator in an $n - 1$ dimensional space, and the induction hypothesis applies. For $\ket{x} \in S^\perp$ we have:

$$\braket{Qx|\lambda_n} = \braket{x|Q\lambda_n} = \lambda_n \braket{x|\lambda_n} = 0$$

which shows that $Q \ket{x}$ is in $S^\perp$ as well.

That means $n - 1$ eigenvectors of $\hat{Q}$ are complete in the $n - 1$ dimensional space $S^\perp$ by our induction hypothesis, and so they are linearly indepdent. Call them

$$\{\ket{\lambda_1}, \ket{\lambda_2}, \ldots, \ket{\lambda_{n-1}}\}$$

As each is an element of $S^\perp$ they are also orthogonal to $\ket{\lambda_n}$:

$$\braket{\lambda_i|\lambda_n} = 0, \qquad\qquad i < n$$

So

$$\{\ket{\lambda_1}, \ket{\lambda_2}, \ldots, \ket{\lambda_{n-1}}, \ket{\lambda_n}\}$$

is a set of n eigenvectors of V, which are linearly independent, and therefore complete in V.