

6	Wed. 10/8 Fri., 10/10	<b>3.1-.2</b> Formalism: Hilbert Space & Observables (Q5.6, 6.2-3) <b>3.3-3.4</b> Formal: Hermitian Operator's Eigenstates & Statistical (Q11) <b>Columbia Rep 3pm in AHoN 116</b>	<b>Daily 6.W</b> <b>Daily 6.F</b>
Study Days Mon 10/13 – Tus 10/14			
7	Wed. 10/15 Thurs 10/16 Fri. 10/17	<b>3.5</b> Uncertainty Principle <b>3.6</b> Dirac Notation (Q5.6)	<b>Daily 7.W</b> <b>Weekly 7</b> <b>Daily 7.F</b>

### Equipment

- Griffith's text
- Printout of roster with what pictures I have
- Whiteboards and pens

### Check dailies

#### Announcements:

- **Exam**
  - **Opportunity:** Fix for HW points by next Wednesday. I've provided plenty of comments to get you started.
- **Columbia**
  - This Friday a representative from Columbia will visit to talk about / answer questions about the 3-2 program. There's no optimal time, but we've scheduled a session- presentation/open house for 3pm – as long as folks are dropping in in AHoN 116. The front end of this will overlap with some folk's classes – come to after; the back end will overlap with practices(?), leave early.

### Daily 6.M Monday 10/6 Griffiths Appendix A.3-.6 Linear Algebra

1. Math: A.8
2. Starting Weekly HW ( A.9)
3. Math: A.14
4. Math A.19
5. Starting Weekly HW ( A.25)

### 3.1 Hilbert Space

- So, we've been doing this whole, 'quantum thing' for a while now, and Griffiths has wisely decided to wait until we've gotten a little, concrete, experience under our belts before casting it all in more general terms. Of course, that second-day reading from Mandl foreshadowed some of this, and so did our early reading of A.1-.2 (might want to skim back over) and Monday's reading of A.3-.6. Also, this is the language and notation that Moore was using from the get-go in Phys 233.
- So, all put together, this is a bit of a review.

- As we know, wave functions represent the state of (our knowledge of) the system; specific operators represent performing specific observations to determine values of properties like position, momentum, energy, etc.
- **Linear Transforms**  
He proposes that wave functions are more generally abstract ‘vectors’ and operators act upon them to perform linear transforms, the same way a matrix acts on a simple vector, as in

$\mathbf{M}\vec{a} = \vec{b}$  some new vector // mathematical function

Or using slightly different notation

$$\hat{M}|a\rangle = |b\rangle$$

Okay, let’s consider a concrete example:

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

and if we operate on the wave function

$$\Psi_n(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t}$$

(a wave function for the infinite square well)

Then

$$\hat{p}\Psi_n(x, t) = \frac{\hbar}{i} \frac{d}{dx} \left( \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t} \right) = \frac{\hbar}{i} \frac{n\pi}{a} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a} x\right) e^{-\frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t} = Y_n(x, t)$$

Which is indeed a new mathematical function, and we could write that like

$$\hat{p}|\Psi_n(x, t)\rangle = |Y_n(x, t)\rangle$$

If we wanted.

- **Inner product**

Now, for complex vectors, as you’re familiar from A.1-.2, Mandl, and Phys 233, you know how we generalize the dot product to be the “inner product”:

In one notation, that’s

$$\vec{a}'\vec{b}$$

where  $\vec{a}' \equiv \vec{a}^*$ , the complex transpose.

In another notation, that’s

$$\langle a|b\rangle$$

In either case, what it gets you is  $\langle a|b\rangle = a_1^*b_1 + a_2^*b_2 + a_3^*b_3 + \dots = \sum_j a_j^*b_j$

For convenience, let’s say we have two functions of position,  $a(x)$ ,  $b(x)$ , then what we’d have is

$$\langle a(x)|b(x)\rangle = a^*(x_1)b(x_1) + a^*(x_2)b(x_2) + a^*(x_3)b(x_3) + \dots = \sum_j a^*(x_j)b(x_j)$$

Now, rather than having a vector with *discrete* values, we two functions with *continuous* values. Then with only a slight bending of our definition, in the continuous limit,

$$\langle a(x)|b(x)\rangle = \int a^*(x)b(x)dx$$

Or

$$\langle b(x)|a(x)\rangle = \int a(x)b^*(x)dx = \left(\int a^*(x)b(x)dx\right)^* = \langle a|b\rangle^*$$

**Normal.** Of course, the function's we're interested in are *normalized wave functions*,  $\Psi_n(x,t)$ .

And being normalized, we mean

$$\int_{-\infty}^{\infty} \Psi_n^* \Psi_n dx = \int_{-\infty}^{\infty} |\Psi_n|^2 dx = 1$$

so in our new notation, that would read

$$\langle \Psi_n | \Psi_n \rangle = 1$$

Also about what hilbert spaces are in the first place [Casey P](#),

ya I would like to get a clearer definition of a Hilbert Space. The book isn't very definitive other than the given equation and that this is home to wave functions. [Kyle B](#),

I agree, going over this would be nice.

In addition, could we briefly go over the Gram-Schmidt procedure [Jeremy](#) (for this one, see appendix A.1,2)

- **Hilbert Space**

- Seeing as we're bent on using the language of linear algebra, and thus thinking of our wave functions as vectors, they need to satisfy some conditions – 'live in a some vector space.'
- **Definition of a Vector Space:** Recall from Appendix A.1, on vectors, that "a vector space consists of a set of vectors together with a set of scalars, which is closed under two operations: vector addition and scalar multiplication (and includes the null vector.)"
- **Normalized Vector Space?:** Now, we wouldn't be able define a vector space with the constraint:  $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$  because the simple sum of two such vectors would clearly no longer satisfy the requirement (at the very least, they'd integrate to 2.
- **Normalize-able Vector Space?** We couldn't even define a space based on the slightly less-restrictive constraint that the functions are *normalize-able* since that wouldn't include the null vector.
- **Square-Integrable Vector Space:** So, the tightest, space-defining constraint we can assert is that they're square-integrable (the integral doesn't blow up.) *That* defines "Hilbert Space."

Again, a concrete example could be the energy eigen functions of the infinite square well:

$$\int_{-\infty}^{\infty} \Psi_n^* \Psi_n dx = \int_{-\infty}^0 0 dx + \int_0^a \left( \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t} \right)^* \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 t} dx + \int_a^{\infty} 0 dx$$

$$\int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) dx = \frac{2}{a} \int_0^a \sin^2\left(\frac{n\pi}{a} x\right) dx = \frac{2}{a} \int_0^a \frac{1}{2} - \frac{1}{2} \cos\left(\frac{2n\pi}{a} x\right) dx = 1$$

And that's what we get for *any* realistic wavefunction (that is to say, one who's square can possibly represent the probability density of a real object.)

### Orthogonal Solutions

Now, another property that our “vectors” have is that, if the two vectors you're taking an inner product of are both solutions to the Schrödinger equation (as opposed to one solution and one operated-upon solution, which yields a new ‘vector’ / function), then not only do you get 1 when you integrate / inner-product them with themselves, but you get 0 when you integrate / inner-product them with each other.

$$\int_{-\infty}^{\infty} \Psi_n^* \Psi_m dx = 0$$

Again, you demonstrated this for the infinite square well.

In our vector notation, that's

$$\langle \Psi_n | \Psi_m \rangle = 0$$

So, just like the  $x, y, z$  coordinate axes, they're not just normal, their orthogonal; they're *orthonormal*.

Writing these together as one expression,

$$\langle \Psi_n | \Psi_m \rangle = \delta_{n,m}$$

### Complete Ortho-Normal Basis Set

For a given Schrodinger equation, the usual rule about solutions to differential equations applies: once you find general solutions, any other solution is a linear combination of these. We usually find the energy eigen-states, and then yes, any other solution is expressible as a linear combination of these solutions. In that sense, these energy eigen states form a complete, ortho-normal basis set for the region of Hilbert space that is solutions to that particular Schrodinger equation.

$$\Psi(x, t) = \sum_n c_n \Psi_n(x, t)$$

Or, using the ortho-normality,

$$\int_{-\infty}^{\infty} \Psi_m^*(x, t) \Psi(x, t) dx = \int_{-\infty}^{\infty} \Psi_m^*(x, t) \sum_n c_n \Psi_n(x, t) dx = \sum_n c_n \int_{-\infty}^{\infty} \Psi_m^*(x, t) \Psi_n(x, t) dx = \sum_n c_n \delta_{n,m} = c_m$$

Written in our special vector notation, that's

$$\langle \Psi_n | \Psi \rangle = c_m$$

"Could we go over when aligned and antialigned spin eigenvectors are supposed to dot to 1 or 0? Maybe also how orthonormality is related to this. I'm a bit confused as to which eigenvectors match up."

[Anton](#)

1. *Math*: Consider the spin eigenvectors (Table Q6.1).
  - a. Show that they are orthonormal.
  - b. Do they live in Hilbert Space? Explain.

## 3.2 Observables

### 3.2.1 Hermitian Operators

How does Griffiths make the connection between observables and operators? Can we go over Example 3.1?" [Spencer](#)

Now, given the association of the wavefunction with the probability density,

$$|\Psi(x)|^2 = \text{Pr}(x)/dx$$

It then made sense that the average position would be

$$\langle x \rangle = \sum x \text{Pr}(x) = \sum x |\Psi(x)|^2 dx \Rightarrow \int x |\Psi(x)|^2 dx$$

And similarly for any other function of  $x$ ,  $f(x)$

$$\langle f(x) \rangle = \sum f(x) \text{Pr}(x) = \sum f(x) |\Psi(x)|^2 dx \Rightarrow \int f(x) |\Psi(x)|^2 dx$$

Now Griffiths went through some work in Chapter 1 to derive that

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = \int \Psi^*(x) \frac{\hbar}{i} \frac{d}{dx} \Psi(x) dx = \int \Psi^*(x) \hat{p} \Psi(x) dx$$

Trivial as it is to say, the expression for average position could be phrased that way too:

$$\langle x \rangle = \int \Psi^*(x) x \Psi(x) dx = \int \Psi^*(x) \hat{x} \Psi(x) dx$$

So he could generally say that the average of any function of  $x$  and  $p$  could be found by sandwiching the appropriate operator in the integral:

$$\langle Q(x, p) \rangle = \int \Psi^*(x) \hat{Q}(x, p) \Psi(x) dx$$

In our new-found vector-matrix notation, that would look like

$$\langle Q(x, p) \rangle = \langle \Psi | \hat{Q} \Psi \rangle$$

Breaking that down into two steps, that's saying you

- you perform the operation  $Q$  upon the "vector" to "transform" into a new vector:
  - $\hat{Q}|\Psi\rangle = |Y\rangle$
- then take the inner product of that new vector with the original vector
  - $\langle \Psi | Y \rangle$

- **Real Observables – Hermitian Operators**

- Now, since the observables are necessarily *real*, we can say that they are their own complex conjugates:

- $\langle Q \rangle = \langle Q \rangle^*$

- That seems like a harmless enough statement. However, that means the same must be true of the integrals that are being used to find them:

$$\langle Q \rangle = \langle Q \rangle^*$$

- $\langle \Psi | \hat{Q} \Psi \rangle = \int \Psi^* \hat{Q} \Psi dx = \left( \int \Psi^* \hat{Q} \Psi dx \right)^* = \int \Psi^{**} (\hat{Q} \Psi)^* dx = \int \Psi (\hat{Q} \Psi)^* dx = \int (\hat{Q} \Psi)^* \Psi dx = \langle \hat{Q} \Psi | \Psi \rangle$   
 $\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$

Now, if we saw this relationship for *matrices* we'd recognize that the definition of a **Hermitian** conjugate, or adjoint, of a matrix Q would be

$$\langle a | \hat{T} b \rangle = \langle \hat{T}^\dagger a | b \rangle$$

$$\vec{a} \mathbf{T} \vec{b} = \mathbf{T}^\dagger \vec{a} \vec{b}$$

The matrix applied to the left vector that has the same effect as its adjoint applied to the right vector in an inner product. The two are generally related by

$$\mathbf{T}^\dagger = \tilde{\mathbf{T}}^*$$

If  $\mathbf{T}^\dagger = \mathbf{T}$  then we call it “self-adjoint” or **Hermitian**.

So we apply the same name here, and say that the operators that correspond to real observables are “Hermitian” (note: seems like a fudge since, with the matrices, there’s an explicit complex conjugation between an matrix and its Hermitian pair, and a matrix would have to be purely real to be equal to its pair and thus be “self-adjoint” or itself a “Hermitian matrix”; however, for the operators, there’s an implicit complex-conjugating that comes with changing position, and somehow that doesn’t count against the operator’s being called “Hermitian.”)

1. *Conceptual*: Explain all the steps in the derivation in eq. 3.19.

$$\langle f | \hat{p} g \rangle = \int_{-\infty}^{\infty} f^* \frac{\hbar}{i} \frac{dg}{dx} dx = \frac{\hbar}{i} \left( f^* g \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{df^*}{dx} g dx \right) = \frac{\hbar}{i} \left( 0 - \int_{-\infty}^{\infty} \frac{df^*}{dx} g dx \right) = \int_{-\infty}^{\infty} \frac{\hbar}{-i} \frac{df^*}{dx} g dx = \int_{-\infty}^{\infty} \left( \frac{\hbar}{i} \frac{df}{dx} \right)^* g dx = \langle \hat{p} f | g \rangle$$

### 3.2.2 Determinate States

Could we go over the derivation of equation 3.22?" [Antwain](#)

Early on, Griffiths pointed out that making the separability assumption, that

$$\Psi(x, t) = \psi(x)\phi(t)$$

Lead us down a path to finding energy “eigen states”. That is to say, for one of these states

$$\sigma^2(E) = \langle (E - \langle E \rangle)^2 \rangle = \dots = \langle E^2 \rangle - \langle E \rangle^2 = 0$$

So there was no spread whatsoever.

Now, he steps back and speaks more generally of such situations. A “determinate” state is one for which a particular kind of measurement’s outcome is perfectly determined – (done correctly) repeating the measurement for identically prepared systems will give identical results.

Casting this in the new and general language, calling  $Q$  the operator and  $q$  the average (and only) value that it returns,

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

Since this is really how we find the average

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

But we’ve just said that for observables the operators are Hermitian, that is, we get the same result if they’re applied to either vector. So we can make this look more symmetric:

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

The only vector that, dotted with *itself* is 0 is the null vector:

$$|(\hat{Q} - q) \Psi\rangle = 0$$

If we look a little more closely beneath the formalism, this argument is that, for

$$\int_{-\infty}^{\infty} |(\hat{Q} - q) \Psi|^2 dx = 0,$$

with an integrand that is inherently symmetric, it must be that the integrand is itself 0, and heck, its square root is zero.

That is to say  $\hat{Q}\Psi = q\Psi$ .

If we were dealing with matrices and vectors, and we had the analogous relation,

$$\mathbf{M}\vec{a} = \lambda\vec{a}$$

We’d call the possible constants *eigen values* and the corresponding vectors *eigen vectors*.

So

**Determinate states are eigenfunctions of the corresponding operators.**

Can we go over Example 3.1?

1. *Starting Weekly HW* (3.6): Consider the operator  $\hat{Q} = \frac{d^2}{d\phi^2}$ , where  $\phi$  is the azimuthal angle in polar coordinates, and the functions are subject to the same boundary condition shown in eq. 3.26. Is this operator hermitian? Find its eigenfunctions and eigenvalues.

"Can we talk about what it means for a spectrum to be degenerate? [Jessica](#)

Example: It's hard to imagine in 1-D, but imagine in 2-D or 3-D; heck, you probably already met this in Stat. Mech. Thermo – imagine a particle in a 3-D box. The simplest case of energy degeneracy is that a particle oscillating in the x direction but flat in the y and z, one oscillating in the y but flat in the x and z, and one oscillating in the z but flat in the x and y all have different momentum vectors, but they could have the same wavelength and so same magnitude of momentum, and same kinetic energy: the energy state would be 3-fold degenerate: 3 energy-eigen states all with the same energy (eigen value).