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

### 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.F Friday 10/10 Griffiths 3.3-3.4 Formal: Hermitian Operator's Eigenstates & Statistical Interp (Q11)

- 1. *Conceptual*: Discuss the relationship between continuous, discrete, quantization, normalization, stationary states, bound states, and scattering states. Which of these correspond to each other?
- 2. *Math*: (3.10) Is the ground state of the infinite square well an eigenfunction of momentum? If so, what is its momentum? If not, *why* not?
- 3. Math: A particle of mass m is bound in the delta function well. What is the probability

that a measurement of its momentum would yield a value between 0 and  $p_0 = \frac{m\alpha}{\hbar}$ ?

- 4. *Starting Weekly HW*: A particle in the infinite square well has the initial wave function  $\Psi(x,0) = Ax(a-x)$ 
  - a. What is  $\Psi(x,t)$  (feel free to quote the example in Ch. 2)?
  - b. What is the probability a measurement of the energy would yield the value  $\frac{4\pi^2\hbar^2}{2}$ ?

$$2ma^2$$

- c. What is the probability a measurement of the energy would yield the value  $\frac{9\pi^2\hbar^2}{2ma^2}?$
- d. What is the probability of measuring the location of the particle at t = 0 to be between 3a/4 and a?

- e. If, at time *t*, you measure the energy to be  $\frac{9\pi^2\hbar^2}{2ma^2}$ , what is the probability of measuring the location of the particle to be between 3a/4 and *a*?
- 5. *Starting Weekly HW*: Griffiths Problem 3.11 (remember the trick from Daily 4.M pr. 1; classically expect  $\frac{p^2}{2m} = K \le E$ )

# **3.3 Eigenfunctions of a Hermitian Operator**

Section 3.3 is giving me the most trouble. I can understand how states can be discrete or continuous, but I can't understand where anything in the equations comes from. The steps to just form out of thin air and I don't get what they are doing." <u>Anton</u>

## Why focus on Eigen functions of Hermitian Operators?

- **Q:** Translating from math lingo to physics lingo, Griffiths had called a state that's represented by an **eigen function** a \_\_\_\_\_\_ state.
  - (**Determinate** as in the outcome of the corresponding type of measurement is completely determined)
- **Q:** In our theoretical model, operating on a quantum object's wave function with a Hermitian Operator corresponds to doing what experimentally?
  - Taking the corresponding measurement.
- **Q:** Why constrain ourselves to only Hermitian Operators?
  - Only they return *real* average values and measured values must be real.

Okay, since we've reasoned that the operators that return measurable must be Hermitian (since the measurable must be real), we focus in on hermitian operators.

Now, when an operator acts upon one of its eigen functions, it returns just the corresponding eigen value and the probability of getting it is 1, i.e., you're in a 'determinate' state. To make that point mathematically,

In generally, for any state

$$\langle q \rangle = \left\langle \psi \left| \hat{Q} \psi \right\rangle = \int \sum c_m^* \psi_m^* \sum \hat{Q} c_n \psi_n dx = \sum \sum \int c_m^* \psi_m^* q_n c_n \psi_n dx = \sum \sum c_m^* c_n q_n \int \psi_m^* \psi_n dx$$
  
=  $\sum \sum c_m^* c_n q_n \delta_{nm} = \sum c_m^2 q_m = \sum \Pr(m) q_m$ 

However, if the state your system is in is an eigen state,

$$\left\langle q\right\rangle = \left\langle \psi_n \left| \hat{Q} \psi_n \right\rangle = \int \psi_n^* \hat{Q} \psi_n dx = \int \psi_n^* q_n \psi_n dx = q_n \int \psi_n^* \psi_n dx = q_n$$

So the average value is just one eigen value and the probability of getting it is just 1. In other words, an eigen state is a determinate (as in measurement result is completely determined) state.

"I am not sure on what it means for eigenvalues to be separated or fill out an entire range. This refers to the definitions of discrete and continuous spectra."

#### <u>Kyle B</u>,

1. *Conceptual*: Discuss the relationship between continuous, discrete, quantization, normalization, stationary states, bound states, and scattering states. Which of these correspond to each other?

As we saw with the infinite square well, the finite square well, the harmonic oscillator, and the delta-function potential, bound systems have **discrete** spectra of separated (countable) eigen values and their vectors are normalizable. In contrast, as we saw with the free particle, and the unbound states of the finite square well and delta function, they have a **continuous** spectra of (uncountable) eigen values and their eigen vectors are not normalizable, thus are *not* in Hilbert Space (though they could be combined as to create normalizable solutions, which then are in Hilbert space.)

#### 3.3.1 Discrete Spectra

He proves two theorem's and asserts one axiom. I'm completely underwhelmed by one, and really impressed by the other proof, and he's clearly over stating the axiom which leaves me wondering what the truly accurate version is.

Theorem 1: Eigenvalues (for bound systems) are real

$$q_{n}\psi_{n} = \hat{Q}\psi_{n}$$

$$\langle\psi_{n}|q_{n}\psi_{n}\rangle = \langle\psi_{n}|\hat{Q}\psi_{n}\rangle = \langle\hat{Q}\psi_{n}|\psi_{n}\rangle = \langle q_{n}\psi_{n}|\psi_{n}\rangle$$
But if it's a Hermitian operator\*
$$q_{n}\langle\psi_{n}|\psi_{n}\rangle = q_{n}^{*}\langle\psi_{n}|\psi_{n}\rangle$$

$$q_{n} = q_{n}^{*}$$

Which means that the eigen values must be real.

**Didn't prove anything we didn't directly build into our model**: we'd actually already reasoned the other way, and more generally: *since* all measured values for *all* wave functions are real, we'd proven that the corresponding operators needed to be Hermitian. Now it kind of goes without saying that, for a *subset of all wave functions* – the eigen functions of the given Hermitian operator – *their measurments* – the eigen values – must be real.

While that previous proof was essentially our taking our initial assumption (real measurable which imply Hermitian operators) and turning it backwards (Hermitian operators imply real measurables), this next proof really has some significance.

Theorem 2: Eigenfunctions (with different eigen values) are orthogonal

Say you have two eigen vectors of the same operator, such that

$$q_n \psi_n = \hat{Q} \psi_n$$
 and  $q_m \psi_m = \hat{Q} \psi_m$ 

Of course, that means that

$$\langle \psi_m | \hat{Q} \psi_n \rangle = \langle \psi_m | q_n \psi_n \rangle = q_n \langle \psi_m | \psi_n \rangle$$
 and  $\langle \hat{Q} \psi_m | \psi_n \rangle = \langle q_m \psi_m | \psi_n \rangle = q_m^* \langle \psi_m | \psi_n \rangle$ 

- But how are  $\langle \psi_m | \hat{Q} \psi_n \rangle$  and  $\langle \hat{Q} \psi_m | \psi_n \rangle$  related?
  - Recall that we'd reasoned

 $\left\langle \psi_{m}\left|\hat{Q}\psi_{m}\right\rangle =\left\langle \hat{Q}\psi_{m}\left|\psi_{m}\right\rangle 
ight
angle$ 

Is true for all operators that yield measurables, and all wave functions that represent particles (are normalizable // are "in Hilbert space"). It was trivial to prove for Q = x and after one integration by parts we prove it for Q = d/dx. Then we suggested but didn't bother to prove that it must be true for all combinations of the two Q(x, d/dx).

So what about  $\left< \psi_m \middle| \hat{Q} \psi_n \right>$  and  $\left< \hat{Q} \psi_m \middle| \psi_n \right>$ ?

- **Problem 3.3** guides one to prove that these are equal. The argument goes like this:
  - say your wave function is a linear combination of two

$$\psi = \psi_m + \psi_n$$

we'll we know it must be true that

(a) 
$$\left\langle \psi \left| \hat{Q} \psi \right\rangle = \left\langle \hat{Q} \psi \left| \psi \right\rangle$$
,

as well as  $\langle \psi_m | \hat{Q} \psi_m \rangle = \langle \hat{Q} \psi_m | \psi_m \rangle$ , and  $\langle \psi_n | \hat{Q} \psi_n \rangle = \langle \hat{Q} \psi_n | \psi_n \rangle$ 

So show what equation plugging  $\psi = \psi_m + \psi_n$  into (a) leaves us with. Call that equation (b)

• Now consider a different linear combination,

$$\xi = \psi_m + i\psi_n$$

By the same reasoning, but being careful about what happens to an i when it's on the left side of an inner product, see what equation that leaves you with; call it (c).

Now add (b) and (c) and you should end up with

$$\left\langle \psi_{m}\left|\hat{Q}\psi_{n}
ight
angle =\left\langle \hat{Q}\psi_{m}\left|\psi_{n}
ight
angle 
ight
angle$$

Which means that

$$q_n \langle \psi_m | \psi_n \rangle = q_m^* \langle \psi_m | \psi_n \rangle$$

Okay, back to the main body of the argument:

The only two ways for  $q_n \langle \psi_m | \psi_n \rangle = q_m^* \langle \psi_m | \psi_n \rangle$  to be true are But *that*'s true only if

q<sub>n</sub> = q<sub>m</sub><sup>\*</sup>,
 o but we already know they must both be real, so
 q<sub>n</sub> = q<sub>m</sub>
 i.e., the two states are degenerate *or*,
 ⟨ψ<sub>m</sub> |ψ<sub>n</sub>⟩ = 0 the two states are orthogonal.

This proves that eigen functions with different eigen values must be orthogonal!

We know this to be true for the infinite square well and for the simple harmonic oscillator, but my money was on it's *not* being true for the finite square well – I actually did the math and got to a point of "surely the k values that satisfy those transidental functions aren't *just right* to make these three integrals (x<0, 0<x<a, and a<x) sum to zero!? So I'd told you that they *weren't* orthogonal. This proof demonstrates that I was wrong. No matter how unlikely the math may seem, eigen states of a bound system *are* orthogonal!

Can we talk about degenerate eigenfunctions?" Spencer

Example: easy to imagine in 3-d infinite square well (as you use to think about a gas Statistical Mechanics) . wave-function undulating along x and flat in y and z, and one undulating along y with same wavelength and flat in z and x will have different momentum vectors, same momentum amplitudes, and same energy – but they're different states. That's degeneracy: different states with the same energy.

"Can we go through a gram-Schmidt orthodontist procedure?" <u>Casey P</u>,

What about the degenerate states? Then the two eigen vectors may *not* be orthogonal. However, assuming we have two, non-orthoganal (but not identical) eigen vectors: g and f, he points out that they can be rephrased as two orthogonal ones by the Gram-Schmidt orthogonalization procedure.

Normalize the first vector:  $\vec{e}_1 = \frac{\vec{f}}{|f|}$ 

Subtract the projection of the second vector in this direction from the second vector and normalize it:

$$\vec{e}_2 = \frac{\vec{g} - \vec{e}_1 \cdot \vec{g}}{\left| \vec{g} - \vec{e}_1 \cdot \vec{g} \right|}$$

If you have yet another vector,

$$\vec{e}_{3} = \frac{\vec{h} - (\vec{e}_{2} + \vec{e}_{3}) \cdot \vec{h}}{\left| \vec{h} - (\vec{e}_{2} + \vec{e}_{3}) \cdot \vec{h} \right|}$$

Generalizing to *function*, the dot products become inner-product integrals.

#### Axiom: The set of eigenfunctions of an observable are **complete**.

- This is an overstatement, but perhaps not by too much. For example, there's no way to build a square between 2a and 3a from solutions to the infinite square well from 0 to a. But in the scheme of things, this might be a very special limiting case.
- I would have assumed that you couldn't build a function that didn't itself respect the boundary conditions that all eigen functions do (like build a cosine from sines), but if you do the math, you actually *can* build a cosine from 0 to a from sines from 0 to a.
- Then again, this clearly doesn't apply to *just* the bound states of systems that don't have an infinite number of them: consider the finite square well, say it's shallow and only has

one bound state – there's no way to make linear combinations of that one bound state to cover all Hilbert space.

- So I reassert that the eigenfunctions of *bound* systems is complete only over the subspace of bound-state solutions to the given Schrodinger's equation.
- Now, it may be that the *complete* set of eignefunctions bound and unbound for a system truly covers all of the Hilbert space of that system's dimensions (still no way for a 1-D wavefunction to span into 3-D).

## 3.3.2 Continuous Spectra

"Can we talk about Dirac Orthonormality because I am confused what it means in terms of equation 3.33."

Jessica Hide responses Post a response

Admin

I agree, this would be very helpful

Mark T, Redlands, CA

l concur <u>Gigja</u>

As we saw for the free particle, the eigen vectors for unbound systems, which have continuous spectra of eigen values, are not normalizable; their inner-product integrals blow up. Yet, he reasons that the eigen values can still be demonstrated to be *real*, the eigen vectors are still *orthogonal (in the dirac-delta sense)* and are still *complete*.

Since we're always concerned with operators of position, momentum, and combinations thereof, he first goes about finding the eigen vectors for the momentum and position operators.

Example 3.2 Momentum eigen vectors

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

Of course, this differential equation is screaming out for an exponential guess:  $\psi_p = Ae^{\zeta x}$ plug it in, and take the derivative:

$$\frac{\hbar}{i}\frac{d}{dx}Ae^{\zeta x} = pAe^{\zeta x}$$
$$\frac{\hbar}{i}\zeta Ae^{\zeta x} = pAe^{\zeta x} \quad \text{or } \zeta = i\frac{p}{\hbar} \text{ so } \psi_p = Ae^{ipx/\hbar}$$
$$\frac{\hbar}{i}\zeta = p$$

Now, this *can't* be normalized; however, we can ask what is the inner product with for two different p's: ((n n'))

$$\left\langle \psi_{p'} \left| \psi_{p} \right\rangle = \int_{-\infty}^{\infty} \psi_{p'}^{*} \psi_{p} dx = A^{2} \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx = A^{2} \frac{\hbar e^{i(p-p')x/\hbar}}{i(p-p')} \bigg|_{-\infty}^{\infty} = A^{2} 2\hbar \frac{\sin\left(\frac{(p-p')}{\hbar}\right)}{(p-p')}$$

You may recognize the fraction from before,

$$\frac{\sin\left(\frac{(p-p')}{\hbar}\infty\right)}{(p-p')} = \pi\delta(p-p')$$

That came from imaging the infinite space were bound at a and –a so  $p = \hbar \frac{n\pi}{2a}$ 

or from

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \qquad \text{and} \qquad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{+ikx} dk$$
  
with  $\frac{(p'-p)}{\hbar}$ 

$$F(\Delta p/\hbar) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\Delta px/\hbar} dx \quad \text{and} \quad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\Delta p/\hbar) e^{+i\Delta px/\hbar} d(\Delta p/\hbar)$$

If we identify

Replacing k

 $\left\langle \psi_{p'} \middle| \psi_{p} \right\rangle = F\left(\Delta p / \hbar\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\Delta p x / \hbar} dx$  then comparing it with the expression we have,  $\langle \psi_{p'} | \psi_p \rangle = A^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx = A^2 \int_{-\infty}^{\infty} e^{-i(\Delta p)x/\hbar} dx$ we can identify that  $f(x) = \sqrt{2\pi} A^2$ 

But then

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\Delta p / \hbar) e^{+i\Delta p x / \hbar} d(\Delta p / \hbar)$$

Means that

$$\sqrt{2\pi}A^{2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left\langle \psi_{p'} \middle| \psi_{p} \right\rangle e^{+i\Delta px/\hbar} d(\Delta p/\hbar)$$

$$\sqrt{2\pi}A^{2}\hbar = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \langle \psi_{p'} | \psi_{p} \rangle e^{+i\Delta px/\hbar} d(\Delta p)$$

The only way our 'function of x' can simply be a constant is if

$$\langle \psi_{p'} | \psi_{p} \rangle = 2\pi A^{2} \hbar \delta(\Delta p) = 2\pi A^{2} \hbar \delta(p' - p)$$

This suggests a handy normalization constant:  $A = \frac{1}{\sqrt{2\pi\hbar}}$  so

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

Then we simply have

$$\langle \psi_{p'} | \psi_{p} \rangle = \delta(p' - p)$$

The normalization constant.

As for the completeness,

We can then say that any solution must be expressible as a linear combination of solutions, but now the sum of solutions must be continuous, i.e., an integral, and so the coefficients of that sum becomes a continuous function.

$$\psi(x) = \int_{-\infty}^{\infty} c(p) \psi_p(x) dp$$

 $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)e^{+ikx}dk$  from chapter 2)

(which is just a rephrasing of  $-\infty$  from chapter So we can pull out the function for the coefficients just as always.

$$\left\langle \psi_{p'}(x) \middle| \psi(x) \right\rangle = \int_{-\infty}^{\infty} c(p) \left( \int_{-\infty}^{\infty} \psi_{p'} \psi_{p} dx \right) dp = \int_{-\infty}^{\infty} c(p) \left\langle \psi_{p'} \middle| \psi_{p} \right\rangle dp = \int_{-\infty}^{\infty} c(p) \delta(p'-p) dp = c(p')$$

Similarly, he demonstrates that the eigen functions for the position operator are orthonormal in the Dirac sense.

Rather trivially,

#### $\hat{x}\psi_x = x\psi_x$

Thinking of this as an eigen value problem, on the one hand, the operator is simply x, on the other hand, an eigen value is a specific value, call it  $x_0$ , so when you "operate" on the eigen function you get this back:

 $x\psi_{x_o} = x_o\psi_{x_o}$ 

The function that does this must be 0 for all x but x<sub>o</sub>:  $\psi_{x_o} = \delta(x - x_o)$ 

Then, for orthogonality:  $\langle \psi_{x_1} | \psi_{x_o} \rangle = \int \delta(x - x_1) \delta(x - x_o) dx = \delta(x_1 - x_o)$ 

Clearly, these functions are obviously complete: they can describe every location along the x axis.

1. *Math*: (3.10) Is the ground state of the infinite square well an eigenfunction of momentum? If so, what is its momentum? If not, *why* not?

## 3.4 Generalized Statistical interpretation

"Can we see an example of the process described in 3.4? Or at least go over that section thoroughly?" <u>Jonathan</u>

Now, we're already familiar with the notion that

$$\langle E \rangle = \sum \Pr(n) E_n$$

$$\langle E \rangle = \left\langle \psi \left| \hat{H} \psi \right\rangle = \left\langle \sum_n c_n \psi_n \left| \hat{H} \sum_m c_m \psi_m \right\rangle \right\rangle = \left\langle \sum_n c_n \psi_n \left| \sum_m c_m \hat{H} \psi_m \right\rangle \right\rangle = \left\langle \sum_n c_n \psi_n \left| \sum_m c_m E_n \psi_m \right\rangle \right\rangle$$

$$= \sum_n \sum_m c_m c_n^* E_n \left\langle \psi_m \left| \psi_n \right\rangle \right\rangle = \sum_n \sum_m c_m c_n^* E_n \delta_{n,m} = \sum_n c_n^2 E_n$$
Where
$$c_n = \left\langle \psi_n \left| \psi \right\rangle \text{ so evidently } c_n^2 = \left| \left\langle \psi_n \left| \psi \right\rangle \right|^2 = \Pr(n)$$

Now, what if we want to know, say, the average position instead? Rather than projecting the wavefunction onto a basis set of the *energy* eigen states, we'd project it onto a basis of the *position* eigenstates. Etc. the difference here is that we're going after a *continuous* function rather than a discrete one, so the 'coefficient' is now a function, and its relation to the

coefficients in the discrete sum is  $c(x_o) = \frac{c_o}{\sqrt{dx}}$ 

$$c(x_o) = \langle \psi_x | \psi \rangle = \int_{-\infty}^{\infty} \delta(x - x_o) \psi dx = \psi(x_o)$$

Then the probability of being in a arrange of x<sub>o</sub>'s is

$$\Pr(x_o < x < x_o + dx) = |c(x_o)|^2 dx = |\psi(x_o)|^2 dx$$

Similarly for momentum,

$$\frac{c_p}{\sqrt{dx}} = c(p) = \left\langle \psi_p \right| \psi \right\rangle = \int_{-\infty}^{\infty} \psi_p^* \psi dx = \int_{-\infty}^{\infty} \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \psi dx \equiv \Phi(p)$$

 $\Pr(p_{o}$ 

- 1. *Math*: A particle of mass m is bound in the delta function well. What is the probability that a measurement of its momentum would yield a value between 0 and  $p_0 = \frac{m\alpha}{\hbar}$ ?
- 2. *Starting Weekly HW*: A particle in the infinite square well has the initial wave function  $\Psi(x,0) = Ax(a-x)$ 
  - a. What is  $\Psi(x,t)$  (feel free to quote the example in Ch. 2)?
  - b. What is the probability a measurement of the energy would yield the value  $\frac{4\pi^2\hbar^2}{2}$ ?

$$\overline{2ma^2}$$

- c. What is the probability a measurement of the energy would yield the value  $\frac{9\pi^2\hbar^2}{2ma^2}?$
- d. What is the probability of measuring the location of the particle at t = 0 to be between 3a/4 and a?
- e. If, at time *t*, you measure the energy to be  $\frac{9\pi^2\hbar^2}{2ma^2}$ , what is the probability of measuring the location of the particle to be between 3a/4 and *a*?
- 3. *Starting Weekly HW*: Griffiths Problem 3.11 (remember the trick from Daily 4.M pr. 1; classically expect  $\frac{p^2}{2m} = K \le E$ )