7	Fri. 10/17	3.6 Dirac Notation (Q5.6)	**Daily 7.F**
8	Mon.10/20 Wed.10/22 Thurs 10/23	4.1.1 -.2 Schrodinger in Spherical: Separation & Angular (Q9.1) 4.1.2-.3 Schrodinger in Spherical: Angular & Radial(Q9.1) Computational: Spherical Schrodinger's	**Daily 8.M** **Daily 8.W** **Weekly 8**

Equipment

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

Check dailies

Announcements:

Daily 7.F Friday 10/15 Griffiths **3.6** Dirac Notation(Q5.6)

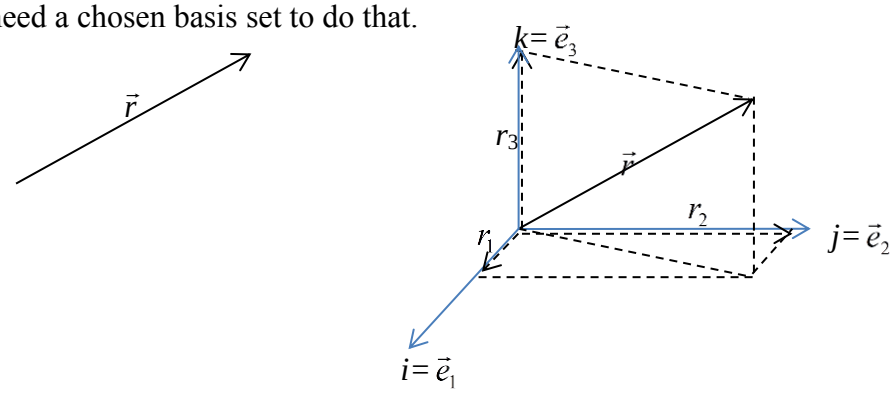
1. *Conceptual/Math*: Let operator $\hat{A}$, representing observable A, have 2 normalized eigenstates ψ_1 and ψ_2, with eigenvalues a_1 and a_2. Operator $\hat{B}$, representing observable B, has 3 normalized eigenstates ϕ_1, ϕ_2, and ϕ_3, with eigenvalues b_1, b_2, and b_3. The eigenstates are related by $\psi 1 = C(2\phi_1 + \phi_2 + 3\phi_3)$ and $\psi 2 = D(3\phi_1 + 2\phi_2 + \phi_3)$.
    a. Can we always write eigenstates of one operator as linear combinations of another eigenstate? Explain.
    b. If observable A is measured to be a_1, what is the state of the system (immediately) after the measurement?
    c. If B is now measured, what are the possible results and what are their probabilities?
    d. Do A and B commute? Explain

3.6 Dirac Notation

Ever since Phys 233, you've been dablinging in Dirac Notation. It's essentially the unification of notation for discrete vectors and matrices with that for functions and operators. I can't honestly say what bit of new *notation* Griffiths introduces in this section, but what he does do is push us think about the states in a basis-set free kind of way, and explicitly crosses over from functions and operators to vectors and matrices. The latter gives us a glimmer of how Dirac connected Shrodinger's wave mechanics with Heisenberg's Matrix mechanics and showed that they were equivalent.

3.6.1 Basis-Free State Vectors

Griffiths draws an analogy to vectors in real space. Consider the separation vector between this room and the chapel – you can picture it, with enough wood you could even construct it, and you don't need a chosen basis set to do that.



Of course, it's often *useful* to select a basis set and project a position vector onto it:

$$\vec{r} = r_1\vec{e}_1 + r_2\vec{e}_2 + r_3\vec{e}_3 = \sum r_n\vec{e}_n$$

This of course has the same basic form as when we write a wavefunction in terms of a basis set of eigenfunctions.

$$\Psi = \sum c_n \Psi_n$$

Or in Dirac notation, we might write

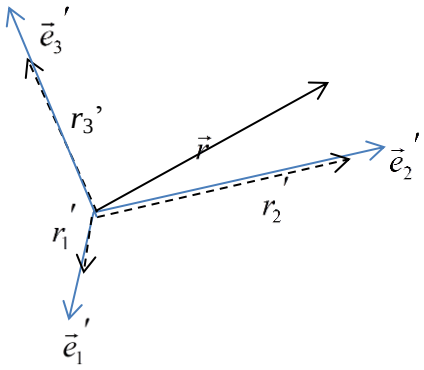
$|r\rangle = \sum r_n |e_n\rangle$ or, for the wave function, maybe $|\Psi\rangle = \sum c_n |\Psi_n\rangle$

For that matter, the individual coefficients are related to the vector and the basis vectors in the same way whether we're talking a position vector or a state vector: each is the inner product of the vector with the respective basis vector

$\langle e_n | r\rangle = r_n$ and $\langle \Psi_n | \Psi\rangle = c_n$

True, since our wave functions are truly continuous *functions*, the "inner product" for them is a generalization (doing the integral) of what it is for vectors with discrete elements, but it's the same idea.

Another similarity between something like the position vector and one of these wave functions is that the *vector* itself is independent of basis set – you can choose another complete basis set and describe it in terms of *that* set instead. For example:



$$\vec{r} = r_1'\vec{e}_1' + r_2'\vec{e}_2' + r_3'\vec{e}_3' = \sum r_n'\vec{e}_n'$$

$$|r\rangle = \sum r_n' \left| e_n' \right\rangle$$

By the same token, you know that the same wavefunction can be rephrased in terms of different complete basis sets – say, energy eigen states, momentum eigen states, and position eigen states.

$$|\Psi\rangle = \sum c_n' \left| \Psi_n' \right\rangle$$

Formally, Griffiths steps back from even specifying the state of the system with a wavefunction in terms of position (what its value is at different positions), and more abstractly says it is in some *state* at a given time

$$|S(t)\rangle$$

That is analogous to the 'separation between room and chapel'

Then it's 'projection' onto a 'position basis set' is what we've commonly just called the (position) 'wave function' – but really how the state varies from one position to another:

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

(as x varies continuously, this 'coefficient' that comes from the inner product is itself a continuously varying function.)

Another way to describe the state is in terms of how momentum eigen states are mixed together to form it, that is, in terms of a momentum basis set, and that's what he's called the momentum wave function:

$$\Phi(p,t) = \langle p|S(t)\rangle$$

Finally, we can specify how the discrete energy states mix together to form the state,

$$c(n,t) = \langle n|S(t)\rangle$$

(though we usually denote it c_n, I'm trying to represent on equal footing with the others, and c_n is another way of saying 'it's a function of n,' though perhaps not a continuous one)

He makes the point that, expressed in terms of position, momentum, or energy states, we have the same *information* in there – we have a simple recipe for translating between these representations without having to know anything additional about the state of the system.

3.6.2 Operator – Matrix Cross-Over

We're already quite familiar that an operator performs a linear transformation, that is, when it operators upon a function it returns a new function (note: while we often operate upon a state's wavefunction, what it returns is a function, but not necessarily a wavefunction representing the state of the system, just another mathematical function.)

For example,

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

For that matter, each function can be represented in terms of some basis set, using very general notation, call the members of the basis set e_n,

"I'm not sure I follow eq 3.80." Kyle B,

$|\alpha\rangle = \sum_n a_n |e_n\rangle$ for discrete or $|\alpha\rangle = \int \left(\frac{da}{dn}\right) e_n dn$ for a continuous distribution

And

$|\beta\rangle = \sum_n b_n |e_n\rangle$

We'll specify that this is an *ortho-normal* basis set, since that's generally what we've been dealing with in position, momentum, and energy states.

Say we know how our initial function, a, is expressed in terms of the chosen basis set, that is, we know all the a_n's, and we want to know how the new function, *b*, is.

Of course,

$$\langle e_m|\beta\rangle = \sum_n b_n \langle e_m|e_n\rangle = \sum_n b_n \delta_{n,m} = b_m$$

Digression: Projection Operator

"Can we talk about what the projection operator does?" Jessica

In general, you have wavevector and you can express it as linear combination of the eigen vectors that define a complete basis set

$$|\alpha\rangle = \sum_n a_n |e_n\rangle$$

For example, when we had funny things like a wave in the form of a triangle and we expressed it as a linear combination of the sinusoidal energy eigen states for an infinite square well.

Of course, if the basis set is *ortho-normal*, then $\langle e_n|\alpha\rangle = a_n$ so

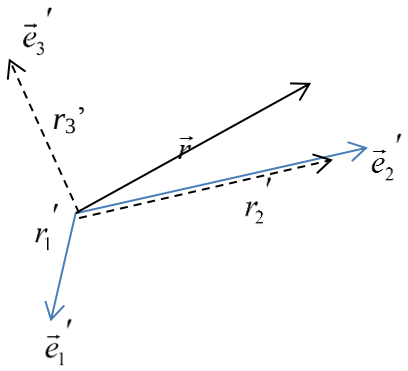
$|\alpha\rangle = \sum_n \langle e_n|\alpha\rangle |e_n\rangle$ He later defines the "Projection Operator" as what you do to

find how much of your given vector lies along another vector, it's projection or shadow on that other vector.
In this case,

$$\hat{P}_{e_n}|\alpha\rangle = \langle e_n|\alpha\rangle |e_n\rangle$$

Similarly, $\hat{P}_{\alpha}|\beta\rangle = \langle\alpha|\beta\rangle|\alpha\rangle$

For a real-space example,



$$\vec{r}_2 = (\vec{r}\cdot\vec{e}_2)\vec{e}_2$$

Back to the main program:
On the other hand,

$$\langle e_m|\hat{Q}\alpha\rangle = \langle e_m|\beta\rangle = b_m$$

$$\sum_n a_n \langle e_m|\hat{Q}e_n\rangle = b_m$$

Now, what exactly *is* $\langle e_m|\hat{Q}e_n\rangle$?

Specific, real-space, example.

Well, let's consider a really explicit example, say we're working in real space and the basis set is just the x, y, and z coordinates and the operator is some sort of linear transformation.

$$\langle e_1|\hat{Q}e_2\rangle = [1,0,0]\begin{bmatrix} Q_{1,1} & Q_{1,2} & Q_{1,3} \\ Q_{2,1} & Q_{2,2} & Q_{2,3} \\ Q_{3,1} & Q_{2,3} & Q_{3,3} \end{bmatrix}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = [1,0,0]\begin{bmatrix} Q_{1,2} \\ Q_{2,2} \\ Q_{2,3} \end{bmatrix} = Q_{1,2}$$

Oh, that just pulls out the m,n^{th} element of the matrix:

$$\langle e_m|\hat{Q}e_n\rangle = Q_{m,n}$$

Phrased a little differently: if you know the functional forms of the eigenvectors and of the operator (say, it's the momentum operator with its derivative) then you can use this relation to fine each matrix element.

$$\sum_n a_n Q_{m,n} = b_m$$

Returning to this point about building the matrix from the wavefunctions and operators, $\left\langle e_m \middle| \hat{Q} e_n \right\rangle = Q_{m,n}$, this is an essential part in Dirac's demonstration that Schrodinger's wave mechanics is equivalent to Heisenberg's matrix mechanics. Let's consider a specific example.

1. **Exercise: (will be HW next time)** Consider the infinite well, for which $\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-n^2 \omega_o t}$ where $\omega_o \equiv \frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2$.
   a. Using equation 3.81, solve for an expression for $p^2_{n,m}$, that is, the n,mth element of the $\hat{p}^2$ matrix that corresponds to applying the operator $\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$. Start populating the matrix with its first 16 elements, 1,1 through 4,4. Aside from being hermitian, there's a name for a matrix that looks like this, what is it? That's a signature of the basis set you're using being eigen states of the operators since it obeys $\hat{A}\left|\alpha_n\right\rangle = a_n \left|\alpha_n\right\rangle$
   b. Do the same but to find the elements of the $\hat{p}$ matrix which corresponds to the operator $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$. Show that the matrix is hermitian by demonstrating that $p_{n,m} = p^*_{m,n}$. Notice that the "trace" of this matrix, i.e., the sum of its diagonal terms, is 0. That's a signature of a measurable who's average is 0.

Since we've moved over to working with discrete linear algebra, it's worth brushing up on the basic moves:

1. *Math*: Compute $< u \mid w >, < w \mid u >,$ and $|< w \mid u >|^2$ for the following vectors:
   a. |u> = [1,-i], |w>=[2i,3]
   b. |u> = [1,-2], |w>=[i,-5]
   c. |u> = [1+i,-2+i], |w>=[i,2-i]

Okay, for some practice working with discrete states and operators that are represented as matrices:

"Can we go through example 3.8? Some of the steps were confusing."
Mark T.

He does straddle the line between general and specific in this example, and that may add the confusion a little.
What are the basic steps?

- Question: how does one of the two possible states time evolve?
- Start with two possible states; for example, they could represent spin alignment.
- Assume that these are *not* energy Eigenstates, but presumably energy Eigenstates could be constructed by a linear combination of them, so build that form.
- "How does Griffiths come up with the Hamiltonian hermitian matrix on page 121?"Spencer If you're taking about pg 133 in the paperback from India then its just part of example 3.8 not something he came up with. I can't find anything else so i don't know...Casey P,
- He makes it up. If this were a 'problem' rather than an 'example', the form of the matrix would have to have been given. Say there's some matrix corresponding to the Hamiltonian (here he's particularly vague – not saying *what* the energy of the system might be like, or so exactly what the matrix should look like, but assuming that it's the same for either state (so the diagonals are the same) and assuming that the off-diagonals are real (what, physically that corresponds to, I'm not sure).
- On the one hand, we know what the energy operator, a.k.a. Hamiltonian, will do to an energy eigenstate – return energy eigen values.
- Now we play the game of assuming we have an eigen value and then solving for what it must be and what the corresponding state must be:
    - Extract the "characteristic equation" from that determinate
    - Solve it for the possible eigen values
    - Chose an Eigen value, return to the matrix equation and solve for how the elements of the eigenvector must be related
    - Normalize the eigen vector
    - Repeat for the other eigen vector
- Back to the big question of how the two possible states time evolve: phrase one of the states as combination of the energy eigen vectors, both of whom time evolve in the familiar way.

These last few steps might look familiar from what you did a few times in Phys 233 with the spin states. If there was a varying magnetic field along the Z-axis, then spin aligned with or against Z would have two different energies. If you start out in a state with spin aligned along the *X* axis, how will it time evolve?

"Also can we talk about what Moore means by 'spin observables'?" Jessica

2. *Starting Weekly HW*: Q6A.2