Quantum Mechanics
Website: www.colorado.edu/physics/phys3220

For an overview and motivation (and a review of useful linear algebra terms, basic statistics, and complex numbers), please take a look at my separate "introductory notes".
I won't cover all that in class, it will provide useful perspective and background!

Q.M. is great fun: interesting, surprising, and sometimes rather weird and mysterious. Philosophers still argue about what it all *means*, but we will (mostly) take a "physicist's view": that the single most essential aspect to learn Q.M. is to learn to calculate (accurate, correct, testable!) experimental outcomes. Issues of interpretation will certainly come too, as we go along! (How can we *not* talk about Schrodinger's cat!?)

Classical mechanics starts with this: given initial conditions of a particle (or system), compute **r**(t), position as a function of time. (Differentiating gives **v**(t), and thus momentum.) Quantum mechanics will also start with initial conditions, and make predictions about observables, but we will NOT start with "position and momentum" (we'll get there soon!) There are other observables too, some more easily accessible to experiment, and easier to work with mathematically. E.g. in the presence of a **B-** field, we can observe effects of the magnetic moment of an atom (or electron), a property associated with the circulation of charge ("current loops"). For a single electron, the circulation or "rotation" is called "spin": the electron has a (measurable) spin. Measuring spin is in some ways analogous to measuring the angular momentum of a spinning top (although HOW we measure it is different in practice.)

Spin is the first quantum property we are going to consider. It might not *sound* simpler than position (in freshman mechanics, angular momentum comes near the end and feels really difficult for most people!) but it turns out to be a great starting point to learn the essentials of QM. Richard Feynman (Nobel-prize winning physicist who unified QM with relativity to construct the theory of QED, over 60 years ago) starts his famous freshman lectures on QM by considering what is in practice the simplest "quantum system" imaginable – a single spinning electron. I like the idea of starting with the simplest system when learning something new. (It's sort of like starting classical mechanics with "point particles and no friction", and then adding in complications bit by bit.)

Our starting point: the Stern-Gerlach exp't:

In 1922, Otto Stern and Walther Gerlach, two young assistants to Max Born, devised an experiment to test one of the earliest predictions of Bohr's quantized model of angular momentum. Here's the basic idea: Atoms are small magnets (because they consist of current loops). They have a magnetic moment vector $\vec{\mu}$ (whose magnitude, μ, tells you how *strongly* magnetic they are, and whose orientation aligns with the angular momentum of the circulating current) If you pass such atoms through a non-uniform B-field, there will be a force on the atoms proportional to a component of their (vector) magnetic moment. (I'll derive this in a sec.) If angular momentum is (classically!) a vector that can point in any direction, then the force will range continuously from a max to a min value (depending on the orientation of the atom) and thus the atoms will "smear out", each feeling a different force. But if angular momentum is "quantized" (as Bohr had postulated), then the force will only take on certain discrete values, and the atoms will come out in one direction or another, but not in a "smear". Turns out their **detailed** predictions were wrong(!) The atoms they used (Silver) have a total of zero orbital angular momentum. (They didn't know that in 1922, they thought the ground state had angular momentum L=1, and thus they expected THREE quantized orientations, so 3 output spots) With L=0, both quantum and classical predictions would predict NO smearing at all. But, they saw the beam split – into TWO spots! The result showed quantization, but was also surprising… and led (after a lot of argument) to the modern theory of Quantum Mechanics.

Although it's not completely essential to the quantum story to come, (I could just claim the final result and go from there) I want to derive the formula for the force on atoms in the Stern-Gerlach (S-G) device. It brings in a few key ideas from E&M and classical mechanics (CM), and is a quick review of some important (but possibly not so familiar) things.

See McIntyre Fig 1.1 for a simplified view of a S-G apparatus. There is a B-field that points (mostly) in the z-direction, but is *inhomogenous* (spatially varying, it's stronger lower down, and weaker higher up) Although the field is complicated, the main variation is also in the "z-direction", so the z- direction is special, it is singled out by this device.

In classical E&M, the potential energy (PE) of a magnetic moment sitting in a B field is given by $U = -\vec{\mu} \cdot \vec{B}$. This is equation 6.34 in Griffith's E&M book, it says that magnetic moments like to line up with B fields – compass needles align with the earth's field! (The minus sign says PE is LOWER when μ aligns with B)

Also in classical mechanics, force $\vec{F} = -\nabla U$, where U means "potential energy". Combining these, for atoms passing through the S-G device:

$\vec{F} = +\nabla \vec{\mu} \cdot \vec{B} \approx \frac{\partial}{\partial z}(\mu_z B_z)\hat{z}$

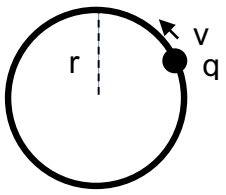
(That last step is approximate – the gradient has x-, y-, and z-components, but most spatial variation in the S-G setup is in the z-direction only, so I'm neglecting x- and y components)

The magnitude of the magnetic moment is a property of the atom, it doesn't vary with space, it's the *B-field that varies*, so $F_z \approx \mu_z \frac{\partial}{\partial z}(B_z)$ is the dominant component of the force. Thus, atoms are pushed "up or down" (in the z-direction) by this S-G. (And the z-component of their little magnetic momen vector decides by how much, and whether it is up or down)

Since we oriented the S-G, we call it a "z- Stern-Gerlach". You could always rotate it by 90 degrees, so the gradient of B is in the x direction, and have an "x- Stern-Gerlach". It's trickier to rotate it to be a "y- Stern-Gerlach" (look at the picture, the poles get in the way of the beams!) but that's a practical issue, not a theoretical one, and we are going to simply idealize these devices and freely talk of S-G's that can be oriented in ANY spatial direction we want!

Now, what's the magnetic moment of a little atom? Griffiths *defines* magnet moment to be μ= IA = current*area. And of course current is merely "charge passing/time taken". If the atom is built out of a charge q rotating in a circular orbit (radius r, velocity v) then

I = q/(time per orbit) = q / (distance around/v) = q/(2 π r/v)
The area here = π r^2, so the π's cancel, and we get: μ= IA = qrv/2.



Magnetic moment points in the direction of the angular moment, **L** = **r**x**p**. Here, L = r*mv, so all together we have $\vec{\mu} = \frac{q}{2m}\vec{L}$.

This was a classical argument for a pointlike mass with charge q in orbit. If the charge was somehow "smeared out" spatially, and the mass was smeared out but *differently*, then we would expect the result to be similar but perhaps with a numerical "fudge factor" out front that takes into account the specific details of this smearing. If the object is e.g. a spinning globe of distributed charge, with "spin angular momentum" **S**, then we have argued that $\vec{\mu} = g\frac{q}{2m}\vec{S}$, where we stuck in the "gyromagnetic ratio" (or gyroscopic ratio) g, it's just a number that accounts for the relative spatial spread of charge and mass.
For point particles in orbit, g=1, as derived above.

Dirac predicted for spinning electrons you would get g=2. (For quarks in a proton, it has yet a different value, because they "smear out" differently) For now the key thing is the proportionality of $\boldsymbol{\mu}$ to spin, **S**. Since "q" = "-e" for electrons, we have as bottom line:

$$F_z \approx -g\frac{e}{2m}S_z\frac{\partial}{\partial z}(B_z)$$

In McIntyre Fig 1.1, dB_z/dz is negative (B gets weaker as you go up the page), so objects with positive S_z will feel an up force, and objects with negative S_z are pushed down.
Of course, if our atom had a net charge, there would be another much bigger force – the good old magnetic F = q**v**x**B** force. That would dominate, and different speed atoms would move different amounts, really smearing everything up. So, we run neutral atoms through S-G's (or build very clever and more complicated versions with e-fields and velocity selectors if you really want to run the experiment with just single electrons!)

McIntyre jumps here to a claim about silver atoms which he attributes to "chemistry" (but is in fact a direct result of the quantum mechanics of atoms! To be covered next semester...) namely, that the electronic structure of silver is this horrible thing:
$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^{10}\,4p^6\,4d^{10}\;\;5s^1$
Remember that notation? The big integers are a principle quantum number, "s, p, d" refer to orbital angular momentum (0, 1, or 2 respectively) and the small superscripts count HOW many electrons live in those particular orbits. So e.g. the $1s^2$ at the start says there are two inner-most electrons each in a "1s" state, which itself has no orbital angular momentum. Never mind the details – it's all a big *closed shell* (total angular momentum and spin ZERO) with ONE lone 5s electron orbiting as the last bit - that means that final outermost electron is an "s-orbit", or zero angular momentum. So the entire magnetic moment of the whole atom arises only from the SPIN of the last electron. It's like we are experimenting on a single electron (except it's neutral! So you can pass it through a B-field *without* it drifting away proportional to the atom's speed, due to the Lorentz force) For this reason, although technically we're working with silver atoms, I tend to think about the S-G device as a device measuring the spin of individual electrons, and will use that language henceforth.

The outcome of the experiment was simple and historically surprising. Electrons (atoms) go up, or down, but nothing else. Since **F** is proportional to S_z, this says the z-component of spin is NOT a continuous variable (I would have classically expected $S_z = |S|\cos\theta$, with θ=the angle of the spin vector - basically ANYTHING, totally random if these things are thermal)

Instead, we only get two possibilities, called "spin-up" or "spin-down". The size of the displacement tells you the magnitude of the spin, and that came out to be $\hbar/2$,
where $\hbar$= "Planck's constant" = $1.05 \cdot 10^{-34}\ J\ sec$

The first quantum surprise here is that the z-component of the spin of electrons is NOT a continuous variable dependent on the "angle" of the spinning electron.
It is quantized, it comes in chunks, discrete possibilities. (Only two of them, here).

The S-G device is called a "spin-analyzer". Whether the particle goes up or down as it exits depends on whether our "measurement" of S_z gave us a result of $\pm\hbar/2$.
So we sometimes say this device is "measuring spin" (although I'd argue you still need a detector to tell you if it went up or down to really be a measurement)

Because of that factor of ½, we call electrons "spin-1/2 objects". (Turns out there are other objects, not electrons, that are "spin-1", or "spin-0", or "spin-3/2", etc.) A spin-1 particle run through a z-S-G device will come out in any of THREE beams.
In general, spin n will produce 2n+1 beams in a S-G. (So all spin-0 objects go straight through – they aren't magnetic!)

FYI, the terminology is that "integer spin" objects are called "bosons", and "half-integer spin" objects (like electrons) are fermions.

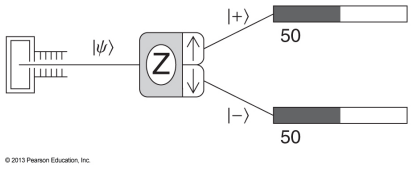
Let's introduce a "quantum language" here – particles are described by their quantum state. Heading in to the S-G, you might have a random (or unknown) state. But after the z-S-G, you know if your particle is spin up ($S_z = +\hbar/2$), or spin down ($S_z = -\hbar/2$). We will call any state a "ket" (I'll tell you why this strange name shortly), and give it a notation like this:

$|\, something\rangle$

That "something" is our choice of a label to describe the state. For a spin-up electron, a natural label might be an up-arrow, or the VALUE of the spin ($+\hbar/2$) or just the SIGN of the spin (+). All of these are ways to remind ourselves of what we know – that the particle's z-component of spin was measured, and we know what it is! Different people might write the "up" output state of a z-S-G (the ones that leaves heading upwards) as $|+\rangle$, or maybe $|+\hbar/2\rangle$, or perhaps $|S_z = +\hbar/2\rangle$, or $|\uparrow\rangle$, or $|+\rangle_z$ (where that little z at the end reminds me that we measured S_z). They are all different names for the same thing.

We often call some generic quantum state ("a ket") $|\psi\rangle$.
Why the word "ket"? Because in math a "bracket" is written like this: $\langle \quad | \quad \rangle$
Since the "ket" is the "right half" of that symbol, it's a "ket'!
Soon we will talk about the "left half", namely $\langle something|$, and call that a "bra".

McIntyre has a nice "Stern-Gerlach" simulator code. It runs in java (which is becoming increasingly challenging to run on new machines) but it's super-helpful. Take some time right now to try to get it running on your computer and play with it. Go to
www.physics.oregonstate.edu/~mcintyre/ph425/spins
You will have to battle with your browser's "permissions" to run java, you can usually dig in and tell it that sims from http://www.physics.oregonstate.edu are safe. Believe in it, you can get it to work! (It will be helpful.) The PhET sim at
https://phet.colorado.edu/en/simulation/stern-gerlach
is ALSO java, and the sim is prettier but not as flexible. Try to get McIntyre's working!



Here is how McIntyre draws a z-S-G device;
The oven is on the left, the incoming state is an unspecified $|\psi\rangle$, the z-S-G is labeled "Z", the output ports are labeled up and down, the outgoing states are labeled $|\pm\rangle$ Those bars at the right are counts – he has run 100 particles through the device, and 50 went up and 50 went down. Apparently, this initial state had a random distribution of z-components of spin. (Of course, if you run the sim, it may come out 52/48, or 47/53, etc… Each individual measurement is *random*, and so the final counts are like what you would get if you tossed a coin 100 times!)

As we move through the book, we'll introduce the basic postulates of quantum mechanics. It may not be obvious that the S-G device contains "all of quantum mechanics", but it does! That's why it's such a helpful way to start learning about QM. The postulates will be consistent with the outcomes of all possible S-G measurements, and in fact all measurements of OTHER observables in quantum systems too. So we start with:

FIRST POSTULATE: the state of any quantum mechanical system is represented symbolically by a "normalized ket", $|\psi\rangle$

There is nothing MORE known about a particle than what is represented in this state. The ket is not "the particle", or "the position of the particle", or "the spin of the particle", it is merely a mathematical object which represents *information about* the particle.

Compare/contrast this with a classical analogy, e.g. $\vec{\boldsymbol{r}}(\boldsymbol{t})$ is not "the particle", but it is "the position of the particle as a function of time", and contains a lot of useful information about the particle – albeit not everything (what about mass, charge, spin, etc…?) For now, our quantum spin-1/2 kets ignore spatial information. We are choosing to inform ourselves about only one component of spin (since that's all that matters for the particular S-G setup we're focusing on right now.) We'll get back to "spatial" information in a couple of chapters!

Since you can orient S-G devices at will, you can imagine lots of experiments that can (and have been) done. The outcomes of some will follow naturally from what we've already seen, but some will contain surprises. Try them out with the SPINS simulator to verify the claims. (Especially helpful if/when you shake your head and say "that surely can't be how it turns out". Remember, this is all experimental outcomes!) Interesting stuff happens when we chain S-G's, so the output of one becomes the input of the next. Running a particle through a S-G "prepares" a quantum state: we can label it, we know what it is, we've measured it.

McIntyre's "Experiment #1" is shown in Fig 1.3 . It's a chain of two "z-S-G's". The output of the + port of the first feeds into the second. Although the starting state was random (half the particles go out the – port of the first S-G) the ones coming out the first + port, have been measured to have $S_z = +\hbar/2$. If you then run them through a second device, you get just what you would expect. These input particles are *known* to be in the state $|+\rangle$, and when you measure S_z on a particle in that state you always get $+\hbar/2$.

No surprise here, no quantum weirdness at all. It's nice to know that if you prepare a state, you know what you've got, and when you measure it again, that's what you still have. Sounds like good physics to me. ☺

Experiment 2 (McIntyre Fig 1.4) Now we chain a z-S-G with an x-S-G. (Notice the "x" label on the second one - the 2nd S-G poles are rotated by 90^o with respect to the first one.) We know the *input state* going into the second analyzer, it's $|+\rangle$, which for emphasis I will write $|+\rangle_z$. What happens after the second analyzer? The experimental outcome is totally random, 50% go "up" (where up now refers to +x, not +z!) and the other half go down. Since we have now measured "x-component of spin", I label the output from the second S-G as $|\pm\rangle_x$, that x-subscript emphasizes what I mean. It's + or – in the x-direction (Maybe I should call it "left or right" instead of "up or down", but hopefully it's clear what I mean.)

This outcome is not weird. By measuring S_z, 1st, we were NOT measuring S_x. If the particles started out random, and we selected out only "spin-z component is up" ones, we haven't (yet) selected out anything about x. The fact that they turn out random in x is not distressing or surprising, I'd say it's expected! The "50/50" split now is just basic spin ½ physics– no matter WHAT direction you orienta S-G, if the input is random (with respect to that axis), the output comes out in only one of two states, "up" or "down" along the axis measured. You could retry exp't 2 using the "z-spin down" beam as input to the second x-SG. You'd get the same result. (Or retry it going into a "y-S-G". Again, same result.)

One last comment, a hint of where we are going – this randomness is very deep. If you run ONE atom through the first S-G (and, say, it happens to come out the + port), then Exp't 2 tells me that the x-component of spin of this object is random. I cannot predict the outcome of one experiment on S-x. If I run many experiments, on average half end up $+_x$, and half $-_x$. But ONE experiment with a 50/50 chance is unpredictable. It is NOT the case that the atom "really has a particular x-spin component but we just don't know it yet". That would be merely a "lack of information". It's deeper than that. If you believed that were true, we could say there is a "local hidden variable", hiding inside the atom, the outcome of the experiment is determined but you and I just don't know it yet. That's a reasonable and classical idea. If I flip a coin but don't reveal it, we firmly (and reasonably) believe it HAS a "heads-or-tails" value, we just don't know it yet. But this prepared spin ½ particle is *different*. It HAS NO VALUE of the x-component of spin until we measure it! That is weird, and you probably don't want to believe me yet. It's hard to think about what it even means. But it is experimentally verifiable, and we shall see the evidence in Chapter 4. For now, let's leave this "interpretation" business be, we're still investigating!

To summarize: if I prepare a particle in state $|+\rangle_z$, and then measure S_z (again), I DO know what the outcome will be (+), but if I instead choose to measure S_x, I do NOT know what the outcome will be. Knowing a state allows you to predict some experimental outcomes with certain, but for others you may only be able to predict probabilities (but not specific outcomes one at a time)

Experiment 3 (McIntyre p. 7) Now we chain three in a row: First Z, then X, then Z. The "+" output of each leads in to the next. Classically, I might say "I measure S_z, then I measure S_x, then I measure S_z again". If you phrase it that way, then since the FIRST measurement of S_z gave us "$+_z$", you might expect the THIRD device (which is also "Z") to give the SAME outcome. But it does not! After measuring S_x, (or phrased more carefully, after exiting an S_x analyzer from the + output port) the results of a subsequent S_z measurement come out 50/50 again. I suppose that too really is expected given our previous experiments. Just as particles with definite S_z come out 50/50 when later measuring S_x, so too particles with definite S_x come out 50/50 when later measuring S_z. The "weird" part is that we thought we know what S_z was (up), only to discover that the result had become randomized. My conclusion would be that measuring S_x impacts or affects the value of S_z. We say these 2 measurements are "incompatible". You cannot know the value of both components of spin for a given particle at one time. If you most recently measured x, you no longer have any knowledge of z. You CAN NOT write down (or prepare) a state $|+_z, +_x\rangle$ (that notation suggests knowledge of both x and z-components of spin) - that would be meaningless and unphysical.

So if I say a particle is "spin up", I mean "the z-component of spin is known, it is $+\hbar/2$. I do not literally mean that the angular momentum points "straight up", because the x (and y-) components are completely undetermined. So quantum mechanical spin doesn't "point" in some clear physical direction. This is sometimes referred to as quantum fuzziness. Again, the state may be well known, the outcome of future experiments is predictable, but SOME experimental outcomes can only be described probabilistically.

Experiment 4: (Figure 1.6) There are 3 variations, all of them chains of 3 S-G's. Setup 4a is the one I just described (Exp't 3). It reiterates that point that if you measure S_x and find $+\hbar/2$, following that with a z-measurement gives you a 50/50 chance of getting + or -. Variant 4b is the same, but using particles that come out of the – port of the S_x analyzer, i.e. the state entering the final analyzer is $|-\rangle_x$. Again, the outcome of the final measurement is 50/50: if you know the "x-state", you do not know the z-value you will get. No surprise here. Variant (c): What if you run BOTH output ports from the middle (X) analyzer back together? (Doing that in practice is subtle. But, with B-fields you can re-steer the beams together. How about building another X-SG and flipping it, mirror reversed, and sticking that just to the right of the middle analyzer, so that you simply "undo" what you just did to the particles?)

If you are thinking classically, you would say "well, I've got particles coming in to the last Z analyser. Half came out the + port of the previous (X) analyzer, and ALL OF THOSE have a 50/50 chance of exiting up or down. (Proven by version a!) Half came out the – port of the previous analyzer, and ALL OF THOSE have a 50/50 chance of exiting up or down (Proven by version b!) So all together, shouldn't we still see a 50/50 output? The answer (surprise!) is no, in this case all particles exit the last Z-analyzer in the same state they exited the first Z-analyzer! (Here, spin up).

If you look at my physical description of how you "recombine" the beams you might get some physical insight into what happened. You undid the first X-analysis, so the "X-SG plus recombining" amounts to "do nothing at all". Thus, if you start with Z-up, you end with Z-up. This suggests that running particles through a S-G is not (yet) a "measurement". It becomes a measurement if there is a way of saying "it definitely went out the upper (or lower) port". The middle S-G in variant (c) is not *measuring* the x-component of spin.

In the SPINS simulator, there's a little button you can push that says "watch". That would be equivalent to having variant (c) with a little counter next to the X-analyzer that says "this particle came out the + port" or "this one came out the – port". If you do that, then you HAVE measured S_x, and you WILL get a 50/50 outcome after the last one, a totally different outcome! In QM, we have to be quite careful when we use the word "measurement", this will come back to bite us if we are too casual about it.

So Exp't 4(c) has some "quantum weirdness". Above, I suggested that running particles through an S_x analyser should randomize S_z, (because we said x- and z-measruements are incompatible) But the recombining of beams shows that the story is subtler than this. Here, we have NOT lost any of the initial information about S_z, even with that S_x device in the middle. But it's not that weird, you have seen something like this effect before, perhaps in Phys 1120, or in Phys 2170. If you shine light through ONE slit, it diffracts and lights up a whole screen. If you shine light through a DIFFERENT slit, offset from the first, it again diffracts and lights up a whole screen. If you shine light through BOTH slits simultaneously, you might think that you would get light from one slit, and add light from the other slight, and thus simply get MORE light everywhere on the screen. But you do not, instead you get bright regions and dark regions, interference patterns! This is NOT quantum mechanics, this is classical wave behavior. Interesting (but not weird). The idea that "combining results from two output ports" gives you something different than "what you would get from one alone, plus what you get from the other alone" might seem weird at first, but it is pretty standard "wave physics". And that's what happens in Experiment 4(c). This suggests there is some "wave physics" buried in our ket notation! (Yes, indeed). We will say that the quantum states of $|+\rangle_x$ and $|-\rangle_x$ can be combined, and as a result can "interfere" with one another. In exp't (c), the state entering the final analyzer is the "coherent superposition" of $|+\rangle_x + |-\rangle_x$, and that, just like a coherent superposition of waves, can give you interesting results!

But I'm getting ahead of myself, we really need to talk about the math of kets a bit more before we can carefully figure out the details of what just happened.

Quantum states:

I cannot tell you what a ket "is". I can only tell you how it behaves mathematically, and how it can be used to predict experimental outcomes (probabilities of measurements). Kets are in *some* ways analogous to vectors. Since right now our spins are all coming out with "two possibilities" (spin-1/2 objects live in a 2-d space) let's have a quick reminder of some properties of good old "2-d" vectors in the plane.

All vectors can be formed as a linear combination of just TWO basis vectors. We get to choose the basis, we normally pick "orthogonal" and "normalized" basis vectors ($\hat{\imath}$ and $\hat{\jmath}$) Since you only need these two basis vectors to construct any other vector, we say this basis is complete. We might change basis (e.g. rotating), That would give a different basis, but still you only need two orthonormal basis vectors. Here's the summary:

$\hat{\imath} \cdot \hat{\imath} = \hat{\jmath} \cdot \hat{\jmath} = 1 \quad (normalization)$

$\hat{\imath} \cdot \hat{\jmath} = \hat{\jmath} \cdot \hat{\imath} = 0 \quad (orthogonality)$

$Any\ \vec{A} = A_x\hat{\imath} + A_y\hat{\jmath} \quad (completeness)$ (McIntyre generalizes to x,y, z space)

The components of **A** can be *computed* by using normalization and orthogonality: dot both sides of the completeness formula with $\hat{\imath}$, for instance, and you find $A_x = \hat{\imath} \cdot \vec{A}$ (Stop, stare, think about that, make sense of it! We will use that "trick" in QM often)

The "dot product" or "inner product" for 2-d vectors doesn't care about ordering, $\hat{\imath} \cdot \vec{A} = \vec{A} \cdot \hat{\imath}$, which won't be true for our generalization to QM.

In QM, kets are in many ways like vectors. The vectors above live in a physical 2-d space. QM kets live in a more abstract "Hilbert" space (but I leave the details of that for your linear algebra course!) Much of what we do with kets can be understood by direct analogy to vectors. So e.g., in our spin-1/2 space, there are also only two basis kets. We get to choose them and usually we will choose the states $|+\rangle$ and $|-\rangle$ as our basis (Those are the "spin up" and "spin down" states from a Z-Stern Gerlach, we call this choice the S_z basis)

Then, *any* general spin ½ quantum state can always be written

$|\psi\rangle = a\,|+\rangle + b\,|-\rangle \quad (completeness)$

"a" and "b" are numbers, they play the same role as the components A_x and A_y above.

One big difference is that a and b can now be *complex* numbers. (I wouldn't know what it means in regular space to have a complex component of a vector! But in Hilbert space that's just what you have)

We still need to define a "dot product" (we'll call it an inner product). If you have a ket $|\psi\rangle$, I can define a corresponding bra which is written $\langle\psi|$, and is defined as

$\langle\psi| = a^* \langle +| + b^* \langle -|$

NOTE! Those coefficients are the *complex conjugates* of a and b. I think of the bra as sort of like the complex conjugate of the ket.

Now I can define an inner product of a bra and a ket, written as a bracket: $\langle bra|ket\rangle$

NOTE! I can't make sense of simply "multiplying" two bras, or two kets. The inner product is "bra on left, ket on right".

Since our basis states are normalized, and orthogonal, and complete, we have

$\langle +|+\rangle = \langle -|-\rangle = 1 \quad (normalization)$

$\langle +|-\rangle = \langle -|+\rangle = 0 \quad (orthogonality)$

$|\psi\rangle = a|+\rangle + b|-\rangle \quad (completeness)$

Stare at those, compare with the corresponding relations for vectors, try to build a mental "analogy" for yourself. Just as an arbitrary vector is a linear combination of $\hat{\imath}$ and $\hat{\jmath}$, so too an arbitrary spin ½ state (ket) is just a linear combination of the basis vectors $|+\rangle$ and $|-\rangle$

Just as I was able to find the components of a vector, so too can I find those coefficients "a" and "b". E.g, "dot" both sides of the completeness relation above on the left with bra $\langle +|$. Try this for yourself, follow the steps!

$\langle +|\psi\rangle = \langle +| (a|+\rangle + b|-\rangle)$

(Here I took the inner product with $\langle +|$ on both sides of the completeness relation above. I added parentheses to guide the eye, but now let's get rid of them. Also, note that the inner product with a sum is the sum of the inner products, inner products "distribute"! So I have:

$\langle +|\psi\rangle = \langle +| a|+\rangle + \langle +| b|-\rangle$

Now, "a" and "b" are just numbers, they can be freely moved around a bracket, so this gives

$\langle +|\psi\rangle = a\langle +|+\rangle + b\langle +|-\rangle$

The first term on the right has a term $\langle +|+\rangle = 1$, the 2nd has $\langle +|-\rangle = 0$ (!), so I get

$\langle +|\psi\rangle = a$.

This is just like $\hat{\imath} \cdot \vec{A} = A_x$ (again, stare at both until you see the analogy! You don't want to have to go through these 3 lines of algebra every single time just to get the "components")

Try taking the inner product of the completeness relation with $\langle -|$, and convince yourself

$\langle -|\psi\rangle = b$

Because of the above 2 results (the formulas to find "a" and "b") , we can rewrite our "completeness" relation in a more formal (but also more general) way which will prove useful later:

Any $|\psi\rangle = \langle +|\psi\rangle \; |+\rangle \;\; + \;\; \langle -|\psi\rangle \, |-\rangle \;\;\;\; (completeness)$

This is the quantum version of saying

Any $\vec{A} = \left(\vec{A}\cdot\hat{\imath}\right)\hat{\imath} + \left(\vec{A}\cdot\hat{\jmath}\right)\hat{\jmath} \;\;\;\; (completeness)$

(Stare for a sec, so you see the connection/analogy)

We can also "flip" the story for bras. Stating with

$\langle\psi| \;\; = \; a^* \langle +| \;\;\; + \;\;\; b^* \langle -|$ and forming the inner product on the RIGHT with $|+\rangle$, convince yourself you get $\langle\psi|+\rangle = \; a^*$. Note the complex conjugate!

This is a big difference between kets and vectors, we used to have

$\hat{\imath}\cdot\vec{A} = \; \vec{A}\cdot\hat{\imath} = A_x$ (order didn't matter, components of vectors are real), but now

$\langle +|\psi\rangle =$ a, but $\langle\psi|+\rangle = \; a^*,$ the order in a bracket does matter, coefficients are complex.

Indeed, this is a general rule: $\langle\varphi|\psi\rangle = \; \langle\psi|\varphi\rangle^*$ If you reverse the order of a bra and ket, you get the compex conjugate.

Our basis vectors are normalized, but in fact all physical kets representing quantum states should be normalized (look back at postulate #1!) This has a consequence for the two complex numbers "a" and "b" in arbitrary states: if $|\psi\rangle = \mathrm{a}\,|+\rangle + \mathrm{b}\,|-\rangle$, then normalization of ψ says $\langle\psi|\psi\rangle = 1$, which means

$(a^*\langle+| + b^*\langle-|)\ (\mathrm{a}\,|+\rangle + \mathrm{b}\,|-\rangle) = 1$

(Sum of two bras on the left, inner product with sum of two kets on the right. Multiply it out, there are 4 terms. Remember that complex numbers can be freely moved out of brackets:

$a^*a\langle+|+\rangle + b^*b\,\langle-|-\rangle + a^*b\langle+|-\rangle + b^*a\,\langle-|+\rangle = 1$

Again, using normalization and orthogonality of the basis kills the "cross terms", and we find $a^*a + b^*b = 1$, or $|\mathrm{a}|^2 + |\mathrm{b}|^2 = 1$

This mathematical relation, true for any state, has a direct physical interpretation (coming very soon!) See McIntyre for an example, or here is another:

Ex: Suppose I want to normalize $|\psi\rangle = \mathrm{A}(3|+\rangle + 4e^{i\pi/4}\,|-\rangle)$

The "A" out front is an unknown number, I want to choose it so ψ is normalized.

Note that that 2nd coefficient is a complex number, written in polar form.

So $1 = \langle\psi|\psi\rangle = A^*\left(3\langle+| + 4e^{\frac{-i\pi}{4}}\langle-|\right)(\mathrm{A}(3|+\rangle + 4e^{\frac{i\pi}{4}}|-\rangle)$

Check for yourself! Forming the bra on the left, I complex conjugated all numbers: A, 3, and $4e^{i\pi/4}$. (The conjugate of 3 is 3, but the conjugate of $4e^{i\pi/4}$ is $4e^{-i\pi/4}$.)

Multiply this all out, again there are 4 terms. Now let's start skipping algebra. The two cross terms (with $\langle+|-\rangle$ or$\langle-|+\rangle$) will contribute zero, and $\langle+|+\rangle = \langle-|-\rangle = 1$, so I really only have two terms that contribute

$1 = \langle\psi|\psi\rangle = A^*A\left(3*3 + 4e^{-i\pi/4}4e^{i\pi/4}\right) = A^*A(9+16) = 25\,|\mathrm{A}|^2$

From that, I conclude A = 1/5.

(I could also add any complex phase to A I want, but I claim that *overall phase of wave functions is not physically meaningful.* We'll see this in a homework problem – it arises from the postulate we are about to introduce)

Now we get to the big punchline, and the reason for all this new math. This is a postulate of Quantum Mechanics, and it is the way we physically interpret all this bra-ket stuff.
The key postulate in QM (McIntyre will add in #2 and #3 shortly!) is:
Postulate #4: If you have a system in state $|\psi\rangle$ and you measure S_z, the probability that you measure one of the two possibilities is $\text{Prob}(\text{measuring } \pm\frac{\hbar}{2}) = |\langle\pm|\psi\rangle|^2$
(We can and will quickly generalize to other measurements, but this is the essence of QM)

EXAMPLES: if your state $|\psi\rangle = |-\rangle$, then
$\text{Prob}(\text{measuring} +\frac{\hbar}{2}) = |\langle+|\psi\rangle|^2 = \langle+|-\rangle^2 = 0$
That makes sense! If you start in the $|-\rangle$ state, we know for sure the measurement will yield $-\frac{\hbar}{2}$, and there is zero chance of measuring $+\frac{\hbar}{2}$!

- If your state $|\psi\rangle = |+\rangle$, then

$\text{Prob}(\text{measuring} +\frac{\hbar}{2}) = |\langle+|\psi\rangle|^2 = \langle+|+\rangle^2 = 1$
That makes sense! If you start in the $|+\rangle$ state, we know for sure the measurement will yield $+\frac{\hbar}{2}$, there is 100% chance of measuring $+\frac{\hbar}{2}$.
Note that we have just "explained" the outcome of Exp't 1 using our new formalism…

- If your state $|\psi\rangle = a|+\rangle + b|-\rangle$, then

$\text{Prob}(\text{measuring} +\frac{\hbar}{2}) = |\langle+|\psi\rangle|^2 = \langle+|\ (a|+\rangle + b|-\rangle)\rangle^2 = |a|^2$
(I had 2 terms to add and then square, but the 2nd one, the one with b in it, vanishes because $\langle+|-\rangle = 0$. Convince yourself!)
Now I have a physical interpretation for a and b: If you start in state $|\psi\rangle = a|+\rangle + b|-\rangle$, then $|a|^2$ is the *probability* that you will measure "spin up", and $|b|^2$ is the *probability* that you will measure "spin up". That's why normalizing states is required, so that $|a|^2 + |b|^2 = 1$ (That's the probability of *either* measuring spin up or spin down added together, which must be 1, because you have to measure one or the other)

We call $\langle+|\psi\rangle$ (which here is "a") the "probability amplitude" for measuring spin up. It is NOT the probability, you must absolute-value-square it to get the probability. It is a complex number. (This reminds me of E&M, where the intensity of a wave, with electric field amplitude E, is $|E|^2$. That's where the language comes from)

For our postulate, we put the "state we have" in the ket, and the "state we want to know the probability of measuring" in the bra. So we write probability amplitudes in the order $\langle out\ (or\ measured)\ state\ |\ input\ state\rangle$ (and then square to get probability)
But this order is just convention, since $=\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$, and probability only cares about the absolute value squared, you could in principle swap the order. We just don't.

Let's continue looking at the 4 Experiments we started off with, and use this math.
We already saw (previous page) that Exp't 1 matches up nicely.

In Exp't 2, we used our first Z-SG spin up output port, and then sent those into an X-SG to measure S_x. We got 50% up (in x), 50% down (in x).
Using postulate 4 (applied to x-measurements now!), I get
Prob(measuring x up, starting with state z up) = $|\langle out|in\rangle|^2 = |\langle +_x|+\rangle|^2 = .5$
Prob(measuring x down, starting with state z up) = $|\langle out|in\rangle|^2 = |\langle -_x|+\rangle|^2 = .5$
Redoing exp't 2 using the spin down output port of the first analyser, we would get
Prob(measuring x up, starting with state z down) = $|\langle out|in\rangle|^2 = |\langle +_x|-\rangle|^2 = .5$, and
Prob(measuring x down, starting with state z down) = $|\langle out|in\rangle|^2 = |\langle -_x|-\rangle|^2 = .5$
I claim these (experimental!) results tell us what the $|+_x\rangle$ state is. Recall, ANY quantum state can be written in the general form $a|+\rangle + b|-\rangle$. So,
$|+_x\rangle = a|+\rangle + b|-\rangle$
$|-_x\rangle = c|+\rangle + d|-\rangle$
Turn those into bras (remembering to conjugate a, b, c, and d!) and plug them into the 4 experimental results above, to find e.g. from the very first one:
$|\langle +_x|+\rangle|^2 = .5 = |a|^2$ (Do it! There is another term involving b^*<-|+>, but that vanishes by orthogonality of |-> and |+>)
The other 3 equations above yield, (in order!) $|c|^2 = |b|^2 = |d|^2 = .5$ (check for yourself)
So I conclude a = c = 1/Sqrt[2]. You *could* put in any complex phase you want (square roots are ambiguous with respect to overall phase) but remember, *overall phase of state vectors is not physically meaningful.*
But we DO have to be careful about the phases of the remaining two (b and d), because we can't just decide all phases MUST be 0. (Only overall phase, not relative phase, is arbitrary)

At this point I can only conclude from the above that
$|+_x\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}e^{i\alpha}|-\rangle$
$|-_x\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}e^{i\beta}|-\rangle$
There are still two undetermined phases, these 4 experiments found 4 probabilities, that's not enough information yet to solve for everything. But we ALSO know that $|\pm_x\rangle$ states are the basis states for the x-component of spin. So THEY should be orthogonal to each other too! That tells us $\langle +_x|-_x\rangle = 0$. Work that out, using the states above. (Do it! Don't forget to complex conjugate the phase in the bra):
$\frac{1}{2}\left(\langle +| + e^{-i\alpha}\langle -|\right)\left((|+\rangle + e^{i\beta}|-\rangle\right)=0$.
Using orthonormality (of the z-basis kets), the two cross terms vanish, and what's left gives $(1+e^{-i\alpha+i\beta})=0$. This says $\alpha - \beta = \pi$. (or 3π, or 5π, etc) This is STILL not enough information to decide both α and β. The reason for that is really that "x" is merely defined so

far as "rotated by 90 degrees from z". There are infinitely many different directions that satisfy this, any arrow in the x-y plane , and that ambiguity amounts to the ambiguity in α. We decide (by fiat) to define which of those to call "x" by choosing $\alpha = 0$. Thus $\beta = \pi$, and:

$$|+_x\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$$

$$|-_x\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle$$

All that complex number stuff just gave us a minus sign in the last term! Our 4 experiments (and some conventions) have given us the S_x basis kets, written in terms of S_z basis kets. You'll use this many times. (McIntyre writes it out in his summary so you can find it easily)

If you want the S_y basis kets, an equivalent set of experiments (using S_y as your second analyzer) will again give you 50/50 outcomes no matter whether you start with + or – in z, giving you (in analogy to the above arguments)

$$|+_y\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}e^{i\alpha}|-\rangle$$

$$|-_y\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}e^{i\alpha}|-\rangle$$

(I have already used orthogonality of these two to get the – sign in the second equation)
But this time we can't just set $\alpha = 0$, otherwise we'd be saying $|+_y\rangle = |+_x$, and that can't be true. How do I know? Run the experiment with chained Y and X S-G's! If you start with $|+_y\rangle$ and then measure S_x, you get 50/50 chance of up or down. (Same with $|-_y\rangle$) The x- and y-basis states are NOT the same. Written using the formalism of Postulate #4, this says $\left|\langle +_x|+_y\rangle\right|^2 = .5$ (and 3 other similar equations, like $\left|\langle +_x|-_y\rangle\right|^2 = .5$, etc)
Since we already know the x-states we can work this bracket equation out – I leave it as an exercise to you, and you should find that

$$|+_y\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{\mathrm{i}}{\sqrt{2}}|-\rangle$$

$$|-_y\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{\mathrm{i}}{\sqrt{2}}|-\rangle$$

Notice that the coefficient on the second ket is complex, but the absolute square of all these coefficients are all 50%.

Let's take a little interlude to talk more about the meaning of this new "symbology".
Consider a particular state you get when you run particles through an X-SG, let's choose the + output port. Those particles are in a definite quantum state we call $|+_x\rangle$
If you measure S_x on such a state you definitely get $+\hbar/2$.
If you measure S_z on such a state, we know you have 50/50 chances of measuring $\pm\hbar/2$.
We have written this above as $|+_x\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$
(Postulate #4 *tells* us this is a 50%/50% mix of "spin up" and "spin down" in z-direction)
This state is called a quantum *superposition of z-spin up and down.*
I think of $|+_x\rangle$ as an equal superposition of "up" and "down" in the z-direction.
Of course, $|-_x\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle$ is ALSO an "equal" superposition of "up" and "down" in the z-direction (Equal, because both coefficients, squared, are .5) but now the minus sign on the second term is giving us a *physically different* state. The relative phase matters!

Classically, you might be tempted to think of "equal superposition" as something like this: "a particle with X-spin "up" has a 50/50 mix of Z-spin outcomes. Maybe it's up, maybe it's down, I just don't know. Like a tossed coin, which could be equally likely heads or tails. But that's not right in QM, because you'd say the same thing about an X-spin "down", and yet we know X-spin "up" and "down" are NOT the same states! I personally prefer to say that a particle with X-spin "up" is z-up AND down, not up OR down! (That's quantum mechanics!)

One issue here is the difference between single particles in the state $|+_x\rangle$ and many similarly prepared particles. We're more familiar with the latter case, where it makes sense to just talk about probabilities. Classically, if I have millions of X-spin "up" particles (and each one is either up or down in z) it's like a pile of tossed coins. Half the measurements of z will reveal up, and half will reveal down. This situation is called a "mixed state": lots of particles, each with a definite Z-value, but we just don't know which value until we look. A mixed state is classical, like a pocket-full of coins. You CAN prepare such quantum states, but they are not so interesting. What is novel in QM is that you can prepare *superpositions*, where EACH particle is NOT "spin-up" or "spin-down", but rather each is a combination of both.

Remember, $|+_x\rangle$ and $|-_x\rangle$ are different states, but either gives the same 50/50 z-outcomes. They are certainly different if you use an X-SG! But they are also different as shown in experiment 4(c). Remember that one? If $|+_x\rangle$ and $|-_x\rangle$ were merely equally MIXED states of z-up and z-down, then when you combined them, you would STILL get an equal mixed state of z-up and z-down. (Right?) But that was NOT the outcome of 4(c)! That's an unambiguous demonstration that superpositions are not just "mixtures". Each particle with state $|+_x\rangle$ is a quantum superposition of z-up and z-down, with a definite PHASE relation between them. Spins are different from coins!
$|+_x\rangle$ is not z-"spin up or spin down", it's z-"spin up AND spin down"!

MATRIX NOTATION:

Bras and kets are essential notation, but it can get clumsy (e.g. taking inner products.) There is a nifty notation we can use to make manipulations simpler and clearer.

In the case of vectors, sometimes I might write $\mathbf{A} \doteq (A_x, A_y)$, an ordered pair of its components. You must have a basis already chosen to make sense of that. And, you can consider that "ordered pair" as a little matrix with just 2 entries. By analogy, *once we have picked our z-spin basis*, we can write our kets in a similar way.

If a ket is $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$, we can write it in shorthand as

$|\psi\rangle \doteq \begin{pmatrix} a \\ b \end{pmatrix}$ That equal with the dot over it is read "is represented by". (It's not literally EQUAL, because if I change basis, the state is NOT changed, the representation changes!)

In this notation, please confirm for yourself that

$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ This is a bit like saying $\hat{\imath} \doteq (1,0)$ and $\hat{\jmath} \doteq (0,1)$

And, similarly, look back at our old results for $|+_x\rangle$ to conclude

$|+_x\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|-_x\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ (Convince yourself!)

Going back to where I showed that if $|\psi\rangle = a\,|+\rangle + b\,|-\rangle$, then $\langle+|\psi\rangle = a$, I would say in full generality that

$|\psi\rangle \doteq \begin{pmatrix} \langle+|\psi\rangle \\ \langle-|\psi\rangle \end{pmatrix}$

That's not really saying anything much different than "the x-component of vector A is $\hat{\imath} \cdot \vec{A}$"

What about bras? In order to get the inner product to be what we want, it's nice and simple if $|\psi\rangle \doteq \begin{pmatrix} a \\ b \end{pmatrix}$, then $\langle\psi| \doteq (a^* \quad b^*)$.

In this way, usual "matrix multiplication" rules give us whatever we want, e.g.

$\langle\psi|\psi\rangle \doteq (a^* \quad b^*)\begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 + |b|^2$

Let's redo some work I skipped above to figure out the representation of $|+_y\rangle$.

The discussion a few pages back led to $|+_y\rangle \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\alpha} \end{pmatrix}$. But I did not work out α.

Let's do it, using the fact that (from experiment, chaining a Y-SG to an X-SG):

$\left|\langle+_x\ |+_y\rangle\right|^2 = .5$ Now we can just plug in our results above…

$\langle+_x\ |+_y\rangle = \frac{1}{\sqrt{2}}(1^* \quad 1^*)\ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\alpha} \end{pmatrix} = \frac{1}{2}(1 + e^{i\alpha})$ (Brackets yield complex numbers!)

Taking the magnitude square of that gives me $.5 = \frac{1}{2}(1 + e^{i\alpha})\frac{1}{2}(1 + e^{-i\alpha})$

Now it's just a bit of (complex) algebra to conclude $cos\alpha = 0$ or $\alpha = \pi/2$, as claimed. (Do it!)

General Quantum States:

Electrons have "spin ½", meaning S_z yields only 2 outcomes, $\pm\hbar/2$. Nature provides us with other particles with spin. Some are also spin ½, but e.g. some mesons have spin 1, and a "Stern-Gerlach"-type experiment would yield only 3 possible outcomes, 0, or $\pm\hbar$.

Particles can have spin "n/2" where n is any integer (and S-G-type experiment then gives only 2n+1 possible outcomes). Integer spin particles are called "bosons", half-integer spin particles are "fermions".

There are other very different measurements of various operators, **A** (being generic now), which yield only a finite range of outcomes, labeled by the n possible eigenvalues of **A**, which we call a_n. (**A** could be e.g., energy for certain systems)

See McIntyre's Fig 1.15 to see a generic depiction of such a system – it's like the S-G picture we always draw, but with n-possible output states.

The generalization of our quantum rules (developed for spin ½) is pretty straightforward.

If our operator **A** has n eigenvalues, it has n basis kets: $|a_i\rangle$ (with i running from 1 to n).

Basis kets are orthonormal and complete: $\langle a_i|a_j\rangle = \delta_{ij} \equiv$ {1 (if i=j), 0 otherwise.}

Any arbitrary state can be written:

$|\psi\rangle = \sum_{i=1}^{n}\langle a_i|\psi\rangle \ |a_i\rangle$ (this is completeness.)

Compare this with the spin ½ formalism, back around p. 13 of these notes!)

Sometimes we call this "expanding a state in a basis". (Do you see why?)

The numerical terms $\langle a_i|\psi\rangle$ (which used to just be called "a" and "b" in spin ½) are sometimes called "expansion coefficients", they are rather like the components of a vector.

Given an initial state $|\psi\rangle$, the probability of *measuring* one of the particular eigenvalues a_n (when you measure **A**) will just be our usual result:

$Prob(a_i) = |\langle a_i|\psi\rangle|^2$

This is the generalization of postulate 4, and provides the physical *interpretation* of the expansion coefficients. They are probability amplitudes: when you square their magnitude you find the probability of making that particular measurement.

You might now take a look (again?) at my "introductory" notes to see a different summary of the story so far, as well as an outline of all the Postulates of quantum mechanics in one place. We are still not ready to present them in their full final/formal wording, we still need a bit more work to set us up.

