3/28/22 Lecture outline

⋆ Books: McIntyre Quantum Mechanics a Paradigms Approach, Cambridge University Press (2023). Feynman Lectures in Physics Volume 3 https://www.feynmanlectures.caltech.edu

⋆ Weeks 1 and 2 reading: McIntyre chapters 1 and 2. Feynman vol 3 chapters 1, 5, 6.

• Hello! What's your name? $|\psi\rangle$: it's Triton the Ket! If you peek at me, we'll become entangled and affect each other. $|\psi\rangle \to |\ddot\smile\rangle$? Maybe.

• Triton the Ket is a vector that lives in a magical space, called Hilbert space, $|\psi\rangle \in \mathcal{H}$. Is $\mathcal{H}$ real? Not exactly. Is it imaginary? Not exactly. Is it complex? Yes, yes it is – literally! The adjoint (think transpose and complex conjugate) of Triton the Ket is Triton the Bra $(|\psi\rangle)^\dagger = \langle\psi| \in \mathcal{H}^\dagger$. Bras and Kets can be combined to get brackets (the names are thanks to Dirac), with $\langle\chi|\psi\rangle = \langle\psi|\chi\rangle^*$ complex numbers; this is like the dot product of two vectors. It follows that the bracket with $\psi = \chi$ (like the dot product of a vector with itself), $\langle\psi|\psi\rangle$, is a real number (which we often set equal to 1).

We can only indirectly see the Triton and $\mathcal{H}$ – if we look too closely, they'll hide from us. $\mathcal{H}$ like a mysterious extra dimension, beyond anything that we can directly see or hear. It's vast, much bigger than all of the space that we know. It encodes the probabilities of all possible outcomes, of our actual world and possibly other alternative realities.

• When you hear the word ket, you should think of a vector in a mysterious space of possibilities. And when you hear the word bra you should think of roughly a complex conjugate of a ket vector. And when you put them together you get a complex number that is like a dot product of the two vectors.

• My UCSD Physics Department Shirt has $\widehat{H}\Psi = E\Psi$, and a picture of the famous cat in a box. The shirt was designed by UCSD physics major Ashley Warner who was also president of UCSD's Undergraduate Women in Physics. I really like this shirt, and I wear it often. Random people sometimes ask me what the equation is, and what it means. We'll spend some time discussing the answers.

• Quantum mechanics is abstract and counter-intuitive, because our intuition is based on a view of Nature that is biased by our large sizes in units of Planck's constant. Gamow's Mr Tompkins (freely available for UCSD ip addresses through the library) imagines how strange things would be if we could move with speeds approaching c, illustrating relativity, and if our size were not so big compared to $\hbar$. I'll discuss dimensional analysis and units, with $v \sim L/T$ and $\hbar \sim \Delta x \Delta p \sim L(ML/T)$. In fact, our modern definitions of some of our units are based on QM properties. I will discuss this a bit later.

• There are two approaches to introduce QM, based on which math class is useful for the system at hand. Systems with a finite number of possibilities, e.g. spin up vs spin down, are governed by linear algebra. Systems with continuous possibilities, like position, are governed by differential equations. In the first case, the equation on my shirt is an eigenvalue equation. In the second case, the shirt equation (SE, which also stands for Schrodinger equation) is a differential equation. The linear algebra version is good for finite dimensional Hilbert spaces (e.g. the energy associated with the electron's intrinsic spin in a magnetic field), whereas the differential equation version is good for infinite dimensional Hilbert space systems. In teaching QM, some books start with the differential equation systems and others start with the linear algebra systems. I like starting with the linear algebra systems, because we can dive right into the quantum weirdness with simpler math. The advantage of infinite-dimensional Hilbert space systems is that they have a classical limit, where some quantum integer $n \to \infty$ (the correspondence principle) and the differential equations look similar to those in wave mechanics (which is why, historically, the triton ψ was called the wave function) though the interpretation (due to Max Born) is that of probability so totally different than usual waves. Starting with the differential equation systems is like tip toeing from our classical everyday experience into Hilbert space whereas starting from the linear algebra systems is like diving right in.

• OK, without further ado, here are the (drumroll please):

The postulates of quantum mechanics

1. The state of the system is given by a ket $|\psi(t)\rangle$. (Not directly measurable!)

2. Physical observables (except time) are replaced with Hermitian operators. The possible measured values of any observable A are the various eigenvalues a_i of the corresponding operator $\widehat{A}$.

3. The probability of measuring that observable A has value a_i in the state $|\psi\rangle$ is $|\langle a_i|\psi\rangle|^2$, where $\widehat{A}|a_i\rangle = a_i|a_i\rangle$ and we have assumed that the eigenvector $|a_i\rangle$ and ket $|\psi\rangle$ are properly normalized, $\langle a_i|a_i\rangle = 1$ and $\langle\psi|\psi\rangle = 1$.

4. After measuring that observable A has value a_i, the measurement itself radically affects the system: the wavefunction (immediately) collapses, $|\psi\rangle \to |a_i\rangle$. This is a bit of an oversimplification and might be discussed more later.

5. The time evolution of the system (aside from the measurement effect above) is given by the Schodinger equation: $i\hbar\frac{d}{dt}|\psi\rangle = \widehat{H}|\psi\rangle$, where $\widehat{H}$ is the Hamiltonian operator.

You can forget about Newton's laws in this class: this equation is all that's needed for determining time evolution. Newton's laws are just an approximation.

• We'll spend the rest of the class explaining and illustrating these postulates.

• The smallest $\mathcal{H}$ that exhibits QM phenomena is a two-dimensional $\mathcal{H}$, meaning that it is spanned by two basis ket vectors. We can write e.g. $|\psi\rangle = \psi_+|+\rangle + \psi_-|-\rangle$ where here $|\pm\rangle$ are some choice of the two basis vectors. Our basis vectors could instead be thought of as $|1\rangle$ and $|0\rangle$ if we think of it as a quantum analog of a computer bit, or as $|\text{ alive}\rangle$ and $|\text{dead}\rangle$ if we think of it as the cat's state. The names $\pm$ could be for example the sign of the spin of an electron along z-axis. Or we could pick a different axis, and that would give some other choice of basis vectors. This is analogous to how ordinary, physical vectors where we can write them with some choice for where we put the (x, y) axes, or some rotated choice, or we could use polar coordinates, etc. The geometric vector doesn't care, but its components depends on the choice of basis. For an ordinary vector we might write $\vec{v} = v_x\widehat{x} + v_y\widehat{y}$, where $v_x = \vec{v}\cdot\widehat{x}$ and $v_y = \vec{v}\cdot\widehat{y}$ if $\widehat{x}$ and $\widehat{y}$ are an orthonormal basis. In Dirac's wonderful notation, we can write this as $|v\rangle = |x\rangle\langle x|v\rangle + |y\rangle\langle y|v\rangle$ since $v_x = \langle x|v\rangle$. In other words, $\mathbf{1} = |x\rangle\langle x| + |y\rangle\langle y|$ and the same equation holds for any orthonormal basis. This is how usual vectors work, and our QM ket vectors are very similar, so in our case of a 2d Hilbert space we can write e.g. $\mathbf{1} = |+\rangle\langle +| + |-\rangle\langle -|$, and then the components in this basis are $\psi_\pm = \langle \pm|\psi\rangle$ and we can write the ket in this basis as $|\psi\rangle(.=)\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}$ (notation).

There are two mathematical differences between QM ket vectors vs usual vectors. One is that everything takes values in the complex numbers, as mentioned above, with $\langle\chi|\psi\rangle = \langle\psi|\chi\rangle^*$. Another is that $|\psi\rangle$ and $c|\psi\rangle$ are the same physically for any complex number c; it is convenient to use this freedom to make $|\psi\rangle$ a unit vector i.e. $\langle\psi|\psi\rangle = 1$ (otherwise various expressions require minor modifications). So we'll take $1 = |\psi_+|^2 + |\psi_-|^2$.

• The ket $|\psi\rangle$ encodes the probability of the all different outcomes. Let's give some examples for the 2d Hilbert space, which arises when there are two different possible outcomes, e.g. spin up or down or cat alive or sad. If $|\psi\rangle = |+\rangle$, then the cat is alive with 100 percent probability. If $|\psi\rangle = |-\rangle$ then the cat is "sad" with 100 percent probability. If $|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ then the probability is 1/2 for each of the two possible outcomes. More generally, the probabilities are

$$P_+ = |\langle +|\psi\rangle|^2, \qquad P_- = |\langle -|\psi\rangle|^2, \qquad \text{with} \qquad P_+ + P_- = 1$$

which makes sense since those are the only two possibilities. It's good that we normalized our ket to be a unit vector since otherwise we'd have to divide the probabilities by $\langle\psi|\psi\rangle$.

• Back to the SE, which we can write as $\widehat{H}|E\rangle = E|E\rangle$, where $\widehat{H}$ is an operator that acts on the Hilbert space, and E is one of its eigenvalues, and $|E\rangle$ is the corresponding eigenvector. An operator is something that maps a ket $|\psi\rangle$ to another ket that we call $H|\psi\rangle$. We always write operators as acting on ket vectors from the left. The operator can also act on bras, and it acts on them from the right e.g. $\langle\psi|H$ is a bra.

• Suppose that you're told that

$$\widehat{H} = E_+|+\rangle\langle+| + E_-|-\rangle\langle-|$$

Then note that $|\pm\rangle$ are eigenvectors of $\widehat{H}$ with eigenvalues $E_\pm$, so in this case we can write $|\pm\rangle = |E_\pm\rangle$. As a matrix, we could write $\widehat{H}$ in this basis as a diagonal matrix, $\widehat{H} = diag(E_+, E_-)$.

• Suppose that we're told instead that

$$\widehat{H} = 17(|+\rangle\langle-| + |-\rangle\langle+|)$$

and we're asked to find the eigenvectors and eigenvalues. Recall in terms of matrices how this is done and compute the eigenvalues for this example.

• It will be important that $\widehat{H}$ is necessarily a Hermitian operator, $\widehat{H} = \widehat{H}^\dagger$ where in terms of matrices $\widehat{H}^\dagger \cong \widehat{H}^{*T}$ transpose complex conjugate (I sometimes denote complex conjugate with a $*$ and sometimes with an overline). Note that that the first example is Hermitian if E_1 and E_2 are real and the second example is Hermitian. We will see that the eigenvalues are the possible values of the energy, and the fact that $\widehat{H} = \widehat{H}^\dagger$ ensures that the energies are indeed real.

• $\widehat{H}$ is called the quantum Hamiltonian. Let's briefly discuss H, the classical Hamiltonian. Notice that we have too many H's, $\widehat{H}$ refer to Hamilton whereas $\mathcal{H}$ refers to Hilbert space. H is the classical version of the quantum $\widehat{H}$. H is a function of the momentum $\vec{p}$, and the positions $\vec{r}$, and its value is basically $E = (KE) + (PE)$. For example, for a non-relativistic particle of mass m with potential energy $V(\vec{r})$, $H = \frac{\vec{p}^2}{2m} + V(\vec{r})$. For example, for a 1d SHO, $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. For a free, relativistic particle of mass m, $H = \sqrt{(c\vec{p})^2 + (mc^2)^2}$; in this class we will ignore relativity and so only treat systems that can be approximated as non-relativistic. This is a pretty good approximation for atomic physics. Combining QM with relativity requires something new: quantum field theory (my research area), which we won't discuss. For time-independent systems, H is a constant of the motion, e.g. for the SHO we have $x_{cl}(t) = A\cos(\omega t + \varphi)$ and plugging in gives $H \to E = \frac{1}{2}m\omega^2 A^2$. The (x,p) space is called phase space and it will come up more in your upper division classical mechanics, and statistical mechanics courses. For the SHO example the classical trajectory is an ellipse in phase space, with size given by A. Classically, A can be anything so E can be anything. As we will see later, QM implies that the only allowed energies are actually the solutions of the differential equation $\widehat{H}\Psi_n \equiv (-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2)\Psi_n = E_n\Psi_n$, and there is only a solution for $E_n = (n+\frac{1}{2})\hbar\omega$, where $n = 0, 1, 2, 3\ldots$ is an integer. In particular, the lowest energy is $\frac{1}{2}\hbar\omega \neq 0$. As we will discuss, there is a quick way to get this from the uncertainty principle $\Delta p \Delta x \geq \frac{1}{2}\hbar$, which roughly says that phase space is pixelated, with pixels of size $\frac{1}{2}\hbar$.

• What's up with the hats? In QM, various physical quantities are replaced by operators acting on the mysterious $\mathcal{H}$. Operator here means that they can act on a ket vector and give a different ket vector. In QM we replace $x \to \widehat{x}$, and $p \to \widehat{p}$ so $H(x,p) \to \widehat{H}(\widehat{x}, \widehat{p})$. For example, for the SHO we have $\widehat{H} = \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega^2\widehat{x}^2$. Angular momentum is also an operator, as is spin (to be discussed). But time t is not an operator. This asymmetry between $(\widehat{x}, t)$ obviously is problematic from the perspective of special relativity, where Lorentz boosted observers can have their time and space coordinates related nontrivially. Aside: in QFT the Lorentz symmetry between space and time is restored by downgrading $\widehat{x}$ to x, and the operator is instead a quantum field that encodes the erstwhile particle.

• Back to our 2d Hilbert space examples. Suppose that we're given some $\widehat{H}$ and we solve for its two eigenvalues E_1 and E_2 and corresponding eigenvectors $|E_1\rangle$ and $|E_2\rangle$. We can choose these eigenvectors to be a complete, orthonormal basis, so we have $\mathbf{1} = |E_1\rangle\langle E_1| + |E_2\rangle\langle E_2|$ and thus $|\psi\rangle = |E_1\rangle\langle E_1|\psi\rangle + |E_2\rangle\langle E_2|\psi\rangle$. Here the system is in a state where the probability of measuring energy E_1 is $P(E_1) = |\langle E_1|\psi\rangle|^2$ and the probability of measuring energy E_2 is $P(E_2) = |\langle E_2|\psi\rangle|^2$.

• Let's connect the abstract math and rules discussed above to a concrete experiment: the Stern-Gerlach experiment. This is discussed in detail in McIntyre and also the Feynman lectures. The experiment demonstrates the quantum principles mentioned above. It also demonstrates that electrons have an intrinsic spin component of angular momentum, $\vec{S}$, which is a 3-component vector and also a Hermitian operator acting in a 2d Hilbert space. It is standard to choose a basis $|\pm$ that diagonalizes S_z and the eigenvalues are $\pm\frac{1}{2}\hbar$. In this basis, we can write $\vec{S} = \frac{1}{2}\hbar\vec{\sigma}$ where $\vec{\sigma}$ are the Pauli matrices:

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that the eigenvalues of all three of these are ± 1 and that all three are Hermitian.

• As a HW exercise you will verify that $[S_x, S_y] = i\hbar S_z$ and you will also verify that $\vec{S}^2$ is proportional to the identity matrix. Note that all of these should have the hats, but I don't want to clutter things with hats above vector arrows. Also, I don't want to have to be consistent with putting hats on every operator, so it'll be good for you to know that operators only sometimes wear their hats and not get too upset if you catch some without their hats.

• The fact that the electron has an intrinsic spin is roughly like it being a little loop of current. A current loop has a magnetic moment, and indeed $\vec{\mu} \equiv g\frac{q}{2m}\vec{S}$ where $q \equiv -e$ is the charge of the electron, m is its mass, and if we thought about it classically we'd obtain $g_{cl} = 1$. Actually g_{expt} is approximately 2 and that is unexplained in QM but was a victory of Dirac's early quantum field theory. The quantum field theory of electrons and light, called QED, is the most precisely verified theory in science because g can be computed by theory and also measured in experiment to amazing precision, (around 1 part in 10^{13}). We'll set $g_e \approx 2$. I remember the value of $\hbar$ by remembering the rhyme $\hbar c \approx 1973 eV \mathring{A}$. More on these units later.

The Stern-Gerlach experiment is to send electrons through an magnetic field and use the fact that there is a force $\vec{F} = -\nabla U$ with $U = -\mu \cdot \vec{B}$ so if $\vec{B} = B_z \widehat{z}$ then

$$F_z \approx \mu \frac{\partial B_z}{\partial z} = -g_e \frac{e}{2m_e} S_z \frac{\partial B_z}{\partial z}.$$

A first shock to a classical physicist is that S_z is not a continuous variable! As we already said, there are only two possibilities $S_z = \frac{1}{2}\hbar$ or $S_z = -\frac{1}{2}\hbar$. The classical physicist expected a smear of electrons in the detector. Instead they arrange in two neat piles, either they go up or they go down! This is an example of why it is called quantum: things that classically are continuous, like angular momentum measured along some axis, are actually quantized!

• Suppose that the electron in a Stern-Gerlach experiment initially had been set up (by Hashem or your favorite name or the initial conditions of the Universe) to have $|\psi\rangle = \frac{1}{5}(3|+\rangle + 4|-\rangle)$. Then if Stern and Gerlach set up their system such that $\partial B_z/\partial z < 0$ (to cancel a minus sign) there would be probability $9/25$ that the electron is deflected up and probability $16/25$ that the electron is deflected down. It is thereafter observed that the measurement affects the system. In short, the wavefunction collapses, so if we observe that it goes up, $S_z = +\frac{1}{2}\hbar$, then $|\psi\rangle \to |+\rangle$ and if we instead observe that it goes down then $|\psi\rangle \to |-\rangle$ immediately thereafter. Explain it, and say some disclaimers.

Things get more interesting once Stern and Gerlach start to measure the beams with a magnetic field first varying in the $\widehat{z}$ direction and then varying in another direction, say the $\widehat{x}$ direction. We can illustrate things more dramatically by considering a measurement where some of the beams are blocked. Suppose we measure first along the $\widehat{z}$ direction and block the electrons that go down. If we measure again along the $\widehat{z}$ direction, all the electrons will go up. So if we block the up ones in the second measurement, then nothing will pass through. But when Stern and Gerlach do the experiment and measure along the $\widehat{x}$ in between, now some electrons do pass through! If the middle measurement for example only keeps the ones that had $S_x = +\frac{1}{2}\hbar$ and now do a third measurement, back to S_z, we'll find that half go up and half go down. The first measurement put the system in an S_z eigenstate, and the second one put it into an S_x eigenstate, and then it is no longer in an S_z eigenstate. Because $[S_x, S_z] \neq 0$, measuring one messes up the other. This is an example of an uncertainty principle: if we're certain about S_z then we're uncertain about S_x and if we're certain about S_x then we're back to being uncertain about S_z. There is a similar phenomenon that happens with light and polarization sheets (next time).

• Define and explain the $P_\pm \equiv |\pm\rangle\langle\pm|$ projection operators, with $1 = P_+ + P_-$ and $P_\pm^2 = P_\pm$ and $P_+P_- = 0$. Mention the book's notation of $\mathcal{P}_\pm$ for probabilities vs $P_\pm$ for projection operators.