Supplementary Notes for lecture 14 for McGill Phys 357.

1. Hilbert Space, Wave Functions, and Zero Eigenvalues

In our derivations so far, we have assumed we have access to a limited number of states (just 2 for spin-1/2 objects). We've said that wave functions have to be properly normalized - *i.e.* $\langle\Psi|\Psi\rangle = 1$. This hasn't been difficult to arrange - nowhere have we seen amplitudes that could go to infinity.

The situation changes quite a lot when looking at a continuous wave function. As an example, consider $\Psi(x)$, a wave function as a function of position. If we were to measure position, there are any number of possible values we might get, and each possible value corresponds to a single state, just like measuring the spin in a Stern-Gerlach machine could give you one of two values. Only, now we have an infinite number of possible values for x. Wave functions must have finite area to correspond to something physical, and this is a huge constraint on potential wave functions. More precisely, a wave function must live in *Hilbert space*. An N-dimensional Hilbert space is the set of all N-element vectors that have a finite inner product. As we take the limit as N goes to infinity, we're left with the set of functions that have finite areas, with every point in infinite-dimensional Hilbert space corresponding to a function with finite area. All valid wave functions must live in Hilbert space.

Much of the challenge of wave mechanics is figuring out, amongst all the solutions to Schrodginer's equation, which solutions live in Hilbert space. Mathematically, wave functions almost always want to blow up as x goes to infinity, unless you pick your solution *very* carefully. We'll see later on that the Schrodinger equation generically ends up looking like

$$\frac{d^2\Psi}{dx^2} = (V(x) - E)\Psi \tag{1}$$

where $V(x)$ is the potential energy as a function of position, and E is the energy of a state. For a state to be bound, the energy has to be less than the potential at large distances, so we're (approximately) left with

$$\frac{d^2\Psi}{dx^2} = V\Psi \tag{2}$$

which has solutions $\Psi = c_- \exp(-\sqrt{V}x) + c_+ \exp(\sqrt{V}x)$. Even if the potential is changing, if you zoom in on a small piece, the potential is nearly-constant, so in that region the wave function is the sum of a growing and a decaying exponential. Over a much larger region, you qualitatively still get a growing and decaying mode. As you move towards infinity, if there is any trace of the growing mode, the solution turns into the exponentially growing one, and your wave function no longer lives in Hilbert space.

The challenge in solving Schrodinger's equation is not just solving the equation, but figuring out which values for the energy give you only the solutions that are decaying at large x. If you change the energy even a little, then you pick up some of the growing solution, and you no longer have a valid wave function. This is generally pretty hard to do, and is why, e.g., it takes a typical textbook an entire chaper to solve the quantum simple harmonic oscillator (SHO).

We'll see the raising and lowering operators return for the SHO. If you can find the raising/lowering operators for your problem, you can find new higher/lower energy states given a single valid wave function. The raising/lowering operators are perfectly happy to keep giving you new states, which might make you think there is an infinite range of possible energies. That does not work, though. For the case of a SHO, there is a minimum energy state, the ground state, and if we try to lower that state, we won't get a valid wave function living in Hilbert space. Since the lowering operator is perfectly happy being applied to the ground state, the only way out of this is if the lowering operator applied to the ground state gives you zero.

We now come back around to the quantization of angular momentum. We saw that the raising/lowering operators applied to a pure state of angular momentum along an axis (say, J_z), return a new state with higher/lower angular momentum along that axis:

$$J_z(J_+ |\lambda, m\rangle) = (m+1)J_+ |\lambda, m\rangle \tag{3}$$

This works if J_+ returns a valid wave function. It also works if J_+ returns 0, because then $J_z(0) = (m+1)(0)$. We know that there's a maximum angular momentum along an axis, because it can't be larger than the total angular momentum. The way we're going to keep all our wave functions living happily in Hilbert space then is if at some point, the raising operator returns zero. If we label the maximum allowed value of m to be j, the only way this happens is if $\lambda = j(j+1)$. We also need the lowering operator to return zero at some point, and if we label that minimum value of m to be j', we saw that $j' = -j$. If we pick any random values of m or λ, we won't get a series of wave functions that terminates. We'll end up with invalid wave functions that don't live in Hilbert space. We can't do that physically, so the only way to get valid solutions is if we pick values for λ *and* values for m such that raising $|\lambda, m\rangle$ enough times brings us to $|\lambda, j\rangle$, and lowering it enough times brings us to $|\lambda, -j\rangle$. If we don't manage both of those things, our raising/lowering operators don't terminate, and we end up with unphysical wave functions.

Because the raising/lowering operators change m by 1 each time, j has to be either an integer or a half-integer, because $j - j'$ is an integer, or $j - (-j) = 2j$ must be an integer. That means, for any system, if we measure the angular momentum along an axis, we always, always get a multiple of $\hbar/2$. Similarly, once we've picked a value for j, then we know that the total angular momentum squared is $j(j+1)\hbar^2$. We aren't free to pick any value for the total angular momentum either. The requirement that our solutions stay physical means that only certain values of angular momentum are allowed - angular momentum *must* be quantized.

2. Simpler Uncertainty Relation

The text works out the uncertainty relation given a commutator, including the possibility of a non-zero expectation value. While that's formally correct, we can safely dispense with the expectations without changing anything important. Essentially, if we have some wave function where we know say the expectation of x is x_0, we just set $x' = x - x_0$, and now the expectation of x' is zero. The variance is the expectation of x'^2. It's identically unchaged from before, but now the math is a lot cleaner. That leaves us applying the Schwarz inequality as follows:

$$\langle\Psi|\mathrm{A}^2|\Psi\rangle \langle\Psi|\mathrm{B}^2|\Psi\rangle \geq |\langle\Psi|\mathrm{AB}|\Psi\rangle|^2 \tag{4}$$

Since the expectations are zero, the left-hand side is the product of the variances of A and B. We rewrite AB as follows:

$$\mathrm{AB} = \frac{\mathrm{AB} + (\mathrm{AB})^\dagger}{2} + \frac{\mathrm{AB} - (\mathrm{AB})^\dagger}{2} \tag{5}$$

As we saw in class, the first term is explicitly Hermitian and the second term is explicitly anti-Hermitian. If both A and B are individually Hermitian, we know that

$$\mathrm{AB} - (\mathrm{AB})^\dagger = \mathrm{AB} - \mathrm{B}^\dagger\mathrm{A}^\dagger = \mathrm{AB} - \mathrm{BA} = [\mathrm{A}, \mathrm{B}] \tag{6}$$

We know that commutators of Hermitian operators are anti-Hermitian because $(\mathrm{AB} - \mathrm{BA})^\dagger = -(\mathrm{AB} - \mathrm{BA})$, and every anti-Hermitian matrix can be written as i times a Hermitian matrix. We can then always write $[\mathrm{A}, \mathrm{B}] = i\mathrm{C}$ for some Hermitian operator C.

This is a long-winded way of saying that the real part of $\langle\Psi|\mathrm{AB}|\Psi\rangle$ is given by $\mathrm{AB} + \mathrm{BA}$ and the imaginary part by $\mathrm{AB} - \mathrm{BA} = [\mathrm{A}, \mathrm{B}]$ (plus factors of 1/2). We can write this even more cleanly by labelling the quantity $\mathrm{AB} + \mathrm{BA}$ the *anti-commutator*, which we write $\{\mathrm{A}, \mathrm{B}\}$. We then have the real part of $\langle\Psi|\mathrm{AB}|\Psi\rangle = \{\mathrm{A}, \mathrm{B}\}/2$ and the imaginary part $[\mathrm{A}, \mathrm{B}]/2$. The absolute value squared is the sum of the real and imaginary parts squared, or

$$|\langle\Psi|\mathrm{AB}|\Psi\rangle|^2 = \frac{|\{\mathrm{A}, \mathrm{B}\}|^2}{4} + \frac{|[\mathrm{A}, \mathrm{B}]|^2}{4} \tag{7}$$

This can never be smaller than the commutator squared, and we only reach equality when the anti-commutator of A and B is zero[1].

We now have our uncertainty relation between A and B in terms of their commutator:

$$\langle\mathrm{A}\rangle^2 \langle\mathrm{B}\rangle^2 \geq \frac{|[\mathrm{A}, \mathrm{B}]|^2}{4} \tag{8}$$

or, taking a square root:

$$\sigma(\mathrm{A})\,\sigma(\mathrm{B}) \geq \frac{|[\mathrm{A}, \mathrm{B}]|}{2} \tag{9}$$

One case we can look at now is angular momentum. Consider a spin-1/2 system in a pure $|+z\rangle$ state. Since $[\mathrm{J_x}, \mathrm{J_y}] = i\hbar J_z$, we know that $\sigma(J_x)\sigma(J_y) \geq \hbar|J_z|/2$. Since we put ourselves into a pure $J_z = \hbar/2$ state with, then $\sigma(J_x)\sigma(J_y) \geq \frac{\hbar^2}{4}$. Since the largest uncertainty we can possibly have along an axis for a spin-1/2 system is $\hbar/2$, then we know that $\sigma(J_x) = \sigma(J_y) = \hbar/2$. Not only that, but since we have equality, that means the anticommutator for a spin-1/2 system $\{J_x, J_y\}$ must be zero, as you can easily verify by multiplying the Pauli matrices.

Of course, other quantities also have commutators. The most famous of these[2] is that $[x, p] = i\hbar$, so we know that $\sigma(x)\sigma(p) \geq \hbar/2$ - better known as the Heisenberg Uncertainty Principle. Energy

[1] We do have to be a little careful here. The commutator doesn't depend on a shift by a constant value, $[\mathrm{A}, \mathrm{B} + \lambda\mathrm{I}] = [\mathrm{A}, \mathrm{B}]$, but the anti-commutator does: $\{\mathrm{A}, \mathrm{B} + \lambda\mathrm{I}\} = \{\mathrm{A}, \mathrm{B}\} + \{\mathrm{A}, \lambda\mathrm{I}\} = \{\mathrm{A}, \mathrm{B}\} + 2\mathrm{A}$. More precisely, if we shift to a space where the means of the operators are zero, we reach equality when the zero-mean anti-commutator is zero.

[2] You'll see on the homework bonus this week that you can derive the angular momentum commutation relations from this by noting that $J = r \times p$.

and time also give rise to an uncertainty relation - $\sigma(t)\sigma(E) \geq \hbar/2$[3]. In the first tiny fraction of a second after the big bang, $\sigma(t)$ couldn't be larger than the age of the universe, so there was a floor on the energy uncertainty of *any* measurement. The energy density of the universe could not have been perfectly uniform just because it wasn't old enough yet for measurements to settle down. We think the universe underwent a phase of exponential expansion called *inflation* very shortly after the big bang, and this expansion froze in the energy fluctuations. These fluctuations gave rise to all the large-scale structure we see in the universe around us, and in fact the details of the structure[4] match what we see today. At a very fundamental level we exist, along with the universe around us, because of quantum uncertainty relations.

[3]There's no actual time operator in quantum mechanics, but once you define what you mean by $\sigma(t)$, then you can show that you get the same energy-time uncertainty relation as you get for position-momentum, etc.

[4]Technically, a Harrison-Zeldovich primordial spectrum