1 Readings

Uncertainty principle: Griffiths, Introduction to QM, Ch. 3.4.

Spin: Griffiths, Introduction to QM, Ch. 4.4; Liboff, Introductory Quantum Mechanics, Ch. 11

2 Heisenberg Uncertainty Principle

Question: Is it possible to construct a quantum state of well-defined position and momentum?

A relevant theorem to help answer the question:

Theorem: Consider two operators $\hat{A}$ and $\hat{B}$ (representing two physical quantities). It is possible to construct a simultaneous eigenstate, ψ_{ab}, of both $\hat{A}$ and $\hat{B}$ iff $[\hat{A},\hat{B}] = 0$ where $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator between $\hat{A}$ and $\hat{B}$.

Proof: i) First, we show that if $[\hat{A},\hat{B}] = 0$, then simultaneous eigenstates exist. Suppose $\{\phi_a\}$ is a set of non-degenerate eigenstates of $\hat{A} \Rightarrow \hat{A}\phi_a = a\phi_a$. Now consider $\hat{B}(\hat{A}\phi_a) = a(\hat{B}\phi_a)$. But, $\hat{B}\hat{A} = \hat{A}\hat{B}$ from the commutator, so $\hat{A}(\hat{B}\phi_a) = a(\hat{B}\phi_a)$. So we conclude that $\psi = (\hat{B}\phi_a)$ is also an eigenstate of $\hat{A}$ with eigenvalue "a". Now if these eigenstates are non-degenerate, then ψ must be a multiple of ϕ, since there can only be one eigenstate with eigenvalue a. Therefore $\psi = \hat{B}\phi_a \propto \phi_a$, i.e., $\psi = \hat{B}\phi_a = b\phi_a$, where b is a constant. Thus b is an eigenvalue of $\hat{B}$. Therefore ϕ_a is a simultaneous eigenstate of $\hat{A}$ and $\hat{B}$. ii) Now we show the converse. If $\hat{A}$ and $\hat{B}$ have simultaneous eigenstates, they are diagonalized by the same transformation, T. Then

$$T^T ABT = T^T ATT^T BT = A^{(D)}B^{(D)} = B^{(D)}A^{(D)} = T^T BTT^T AT = T^T BAT$$

whence we have $AB = BA$. So it the two operators have simultaneous eigenstates, they commute.

So, to answer the question of whether we can construct a state of well-defined position AND momentum, then we must see if $[\hat{x}, \hat{p}] = 0$ or not.

We will evaluate the commutator in the position representation, i.e., in the continuous basis $|x>$ where $\hat{x} = x$ (meaning the position operator is just *the function* x), We previously derived $\hat{p}$ in this position representation as

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}.$$

Let's first test this operator $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ on an test state:

$$\hat{p}\psi_k(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\left(e^{ikx}\right) = \hbar k e^{ikx} = p\psi_k(x).$$

Now we can explicitly calculate the commutator in this basis:

$$\left[x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right] = ?$$

Notice the commutator is itself an operator, in this case one that is asking to operate on some function. Let's apply it to a test function $f(x)$ and see what happens:

$$\left[x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right] f(x) = \frac{\hbar}{i}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right) f(x) = \frac{\hbar}{i}\left(x\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(xf(x))\right) = \frac{\hbar}{i}\left(x\frac{\partial f}{\partial x} - f(x) - x\frac{\partial f}{\partial x}\right) = i\hbar f(x)$$

We see that the test function $f(x)$ is irrelevant and we find

$$[\hat{x}, \hat{p}] = i\hbar \neq 0.$$

Therefore we can conclude that you cannot simultaneously know the position and momentum of a quantum state with certainty. This is one statement of the Heisenberg Uncertainty Principle. This is often stated quantitatively, as

$$\Delta x \Delta p \geq \hbar/2$$

where $(\Delta A)^2$ is the variance of operator A, i.e., $\left\langle (A - < A >)^2 \right\rangle$. Note that the variance is defined for a particular state. Similar uncertainty relations hold between all pairs of non-commuting observables. In your homework this week you prove the general quantitative form of the uncertainty relation between non-commuting observables A and B.

2.1 Uncertainty principle and two-slit experiment

The uncertainty principle is responsible for one of the basic features of the two-slit experiment, namely that if one can observe an interference pattern, that one has no knowledge of which slit the particle went through, while if one measures which slit was traversed, then one looses the interference pattern. Figure 1 shows such a two-slit experiment for a beam of electrons incident from the left. The interference pattern is observed on a scintillation screen on the right. Now suppose we put a source of photons after the slits which will interact with the electrons and allow us to find out ('measure') which slit each electron passed through. In order for this information to be achieved, the position of each electron has to be measured within $d/2$, i.e.,

$$\Delta y \ll \frac{d}{2}.$$

Now if the interference pattern is to be maintained, then the uncertainty in electron momentum induced by the interaction with a photon, Δp_y, must be very much less than a value that would displace the electron from a maximum in the interference pattern to an adjacent minimum. This condition is readlily obtained from trigonometric analysis in Figure 1, giving

$$\Delta p_y \ll \frac{\theta}{2} p_x.$$

But we know from the de Broglie relation that $p = h/\lambda$, and the angle θ at which the first interference maximum occurs is given by the path length difference between the 2 slits, just like diffraction analysis (see Figure 2). Thus $\lambda = d \sin\theta \simeq d\theta$. Hence we have

$$\Delta p_y \ll frach2d$$

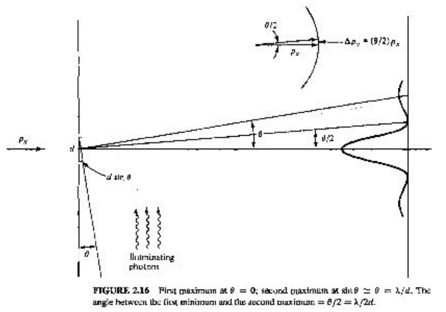

Figure 1: Two-slit experiment

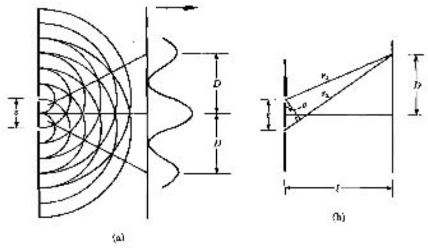

Figure 2: Diffraction - path length difference at first diffraction peak

So now we have derived two inequalities that need to be satisfied if we can both determine which slit the electrons passed through *and* maintain an interference pattern. Combining these two inequalities leads to

$$\Delta y \Delta p_y \ll \frac{h}{4}.$$

Looks good?? NO - this is in direct contradiction to the Heisenberg uncertainty relation for position and momentum! (The numerical factor of π is not meaningful quantitatively, can be fixed by appropriate definition of the uncertainty.) So we have to conclude that it is not possible to both measure which slit was traversed and maintain the interference pattern.

3 Spin

3.1 Physical qubits

Now, after this foray into the world of wave mechanics, let's get back to our discussion of *qubits* (it is in the title of the course, after all!). How can we make a qubit in real life? We need a quantum mechanical two-level system such that we can:

(1) Initialize the qubit.

(2) Manipulate the qubit (think gates!)

(3) Measure the qubit.

There are many other important issues such as decoherence and entanglement, but we'll mainly be focusing on these first three.

Examples of some possible 2-level systems are spins, atoms, photons, superconducting loops. Over the next few lectures we'll be discussing how to physically prepare, measure, and manipulate real qubit systems made from spins.

3.2 Recall what is spin?

Elementary particles and composite particles carry an intrinsic angular momentum called spin. For our purposes, the most important particles are electrons and protons. They each contain a little angular momentum vector that can point up $|\uparrow>$ or down $|\downarrow>$. The quantum mechanical spin state of an electron or proton is thus $|\psi>=\alpha|\uparrow>+\beta|\downarrow>$. Therefore, spins can be used as qubits with $|\uparrow>=|0>$, $|\downarrow>=|1>$.

How do we understand the details of spin? We gave a brief overview of the history and role of classical thinking in the development of spin in lecture 2. Please look back at this before proceeding. The spin angular momentum was shown there to be related to an intrinsic magnetic moment that accounted for an aomalous splitting of energy levels of hydrogen atoms in a magnetic field. It is a relativistic effect that can be derived from the Dirac Equation (Relativistic Schrodinger equation for spin-$\frac{1}{2}$ particles), but it holds for electrons that are not moving fast.

The intrinsic angular momentum is called "spin" = $\vec{S}$, and it is related to the intrinsic magnetic moment by $\vec{\mu}=-\frac{ge}{2m}\vec{S}$. Here g (the g-factor) is a unitless factor. For electrons, $g\approx 2$. For protons, $g\approx 5.6$. You should also note that $\frac{m_{proton}}{m_{electron}}\approx 2000$, so we conclude that $\mu_{\vec{proton}}\ll\mu_{elec\vec{t}ron}$. Note that an electron with orbital angular momentum gives rise to a magnetic moment $\vec{mu}=-\frac{e}{2m}\vec{L}$, so the g-factor can be viewed as a kind of correction factor due to quantum mechanics.

To understand spin = $\vec{S}$ we must first understand the QM properties of angular momentum. Classically, angular momentum is $\vec{L}=\vec{r}\times\vec{p}=\hat{L_x}\mathbf{i}+\hat{\mathbf{L_y}}\mathbf{j}+\hat{\mathbf{L_z}}\mathbf{k}$ where $\mathbf{i},\mathbf{j},\mathbf{k}$ are the usual cartesian unit vectors. To understand angular momentum in QM, we turn the classical observables into *operators* and study the "algebra" of $\vec{L}=\vec{r}\times\vec{p}$ in QM.

Again, and we can't stress this enough, electron spin is not orbital angular momentum in the classical sense. Experiments tell us, however, that we can take most general properties we derive for the QM operator $\vec{L}=\vec{r}\times\vec{p}=\hat{L_x}\mathbf{i}+\hat{\mathbf{L_y}}\mathbf{j}+\hat{\mathbf{L_z}}\mathbf{k}$ and we can simply apply them to the operator $\vec{S}=\tilde{S_x}\mathbf{i}+\tilde{\mathbf{S_y}}\mathbf{j}+\tilde{\mathbf{S_z}}\mathbf{k}$. This is the standard treatment.

Here are some properties that are straightforward to derive for $\vec{L}=\vec{r}\times\hat{P}$, and will be applied here directly to the operator $\vec{S}$. (We will skip the derivations, but they are done in standard texts.)

There are really four important operators associated with spin: $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\vec{S}^2=\hat{S}_x{}^2+\hat{S}_y{}^2+\hat{S}_z{}^2$. *All spin properties* are determined by the commutators between these operators (recall $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$):

$$[\hat{S}_x,\hat{S}_y]=i\hbar\hat{S}_z,[\hat{S}_y,\hat{S}_z]=i\hbar\hat{S}_x,[\hat{S}_z,\hat{S}_x]=i\hbar\hat{S}_y,[\hat{S}^2,\hat{S}_i]=0$$

What are the implications of these commutation relations? First notice that $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ don't commute with each other. Following the results of the last lecture, we conclude that we cannot find a simultaneous eigenstate of any pair of these quantities.

This is strange! We can't know precise values of $\hat{S}_x$ and $\hat{S}_y$ for *any state*. This is just like $\hat{p}$ and $\hat{x}$. Mathematically we can state this by saying that there is no state $|s_x,s_y>$ such that $\hat{S}_x|s_x,s_y>=s_x|s_x,s_y>$ AND $\hat{S}_y|s_x,s_y>=s_y|s_x,s_y>$.

However, notice that $\hat{S}^2$ commutes with any one component of $\vec{S}$. Therefore, we *can* know the precise value of $\vec{S}^2$ and $\hat{S}_i$ for a single component of $\vec{S}$. Following standard convention, let's pick $S_i=S_z$. So we can find spin states $|s,m>$ that are simultaneous eigenstates of $\vec{S}^2$ and $\hat{S}_z$.

$$\hat{S}^2|s,m>= a_s|s,m>, \hat{S}_x|s,m>= b_s|s,m>, a_s, b_m = constants$$

Now our task is to understand spin eigenstates $|s,m>$. First, what are allowed values of a_s, b_m? These are eigenvalues of operators S^2 and S_z representing observables.

Answer:

a can equal $\hbar^2 n(n+1)$, where n is an integer or half of an integer Given that $a = \hbar^2 n(n+1), b$ can equal $\hbar(-n), \hbar(-n+1), \ldots \hbar(n-2), \hbar(n-1), \hbar n$.

Now, let's prove it.

First, we define the somewhat odd (at first glance) "raising" and "lowering" operators S_+ and S_-: $S_+ \equiv S_x + iS_y$, $S_- \equiv S_x - iS_y$

Let's find the commutators of these operators:

$[S_z, S_+] = [S_z, S_x] + i[S_z, S_y] = i\hbar S_y + i(-i\hbar S_x) = \hbar(S_x + iS_y) = \hbar S_+$

Therefore $[S_z, S_+] = \hbar S_+$. Similarly, $[S_z, S_-] = -\hbar S_-$.

Now act S_+ on $|a,b\rangle$. Is the resulting state still an eigenvector of S^2? If so, does it have the same eigenvalues a and b, or does it have new ones?

First, consider S^2:

What is $S^2(S_+|a,b\rangle)$? Since $[S^2, S_+] = 0$, the S^2 eigenvalue is unchanged: $S^2(S_+|a,b\rangle) = S_+(S^2|a,b\rangle) = S_+(a|s,m\rangle) = a(S_+|a,b\rangle)$. The new state is also an eigenstate of S^2 with eigenvalue a.

Now, consider S_z:

What is $S_z(S_+|a,b\rangle)$? Here, $[S_z, S_+] = \hbar S_+ (\neq 0)$. That is, $S_z S_+ - S_+ S_z = \hbar S_+$. So $S_z S_+ = S_+ S_z + \hbar S_+$, and:

$$\begin{aligned} S_z(S_+|a,b\rangle) &= (S_+ S_z + \hbar S_+)|a,b\rangle \\ &= (S_+ b + \hbar S_+)|a,b\rangle \\ S_z(S_+|a,b\rangle) &= (b+\hbar) S_+|a,b\rangle \end{aligned}$$

Therefore $S_+|a,b\rangle$ *is* an eigenstate of S_z. But S_+ raises the S_z eigenvalue of $|a,b\rangle$ by $\hbar$! S_+ *changes* the state $|a,b\rangle$ to $|a, b+\hbar\rangle$.

so S_+ raises the S_z eigenvalue of $|s,m\rangle$ by $\hbar$!

Similarly, $S_z(S_-|s,m\rangle) = (b-\hbar)(S_-|a,b\rangle)$ (Homework.) So S_- lowers the eigenvalue of S_z by $\hbar$.

Now, remember that $\vec{S}$ is an angular momentum. S^2 represents the square of the magnitude of the angular momentum; and S_z represents the z-component.

But suppose you keep hitting $|s,m\rangle$ with S_+. The eigenvalue of S^2 will not change, but the eigenvalue of S_z keeps increasing. If we keep doing this enough, the eigenvalue of S_z will grow larger than the square root of the eigenvalue of S^2. That is, the z-component of the angular momentum vector will in some sense be larger than the magnitude of the angular momentum vector.

That doesn't make a lot of sense . . . perhaps we made a mistake somewhere? Or a faulty assumption? What unwarranted assumption did we make?

Here's our mistake: we forgot about the null state 0, which *acts like* an eigenvector of any operator, with any eigenvalue. This is not the state $|0\rangle$; it is a null state state, equal to 0. For instance, if we were dealing with qubits, any ket could be represented as the $\alpha|0\rangle + \beta|1\rangle$. What state do you get if you set both α and β to 0? You get 0, which is not the same as $|0\rangle$. In other words, you annihilate the ket.

Remember in our proof above when we concluded that $S_z(S_+|a,b\rangle) = (b+\hbar)S_+|a,b\rangle$? Well, if $S_+|a,b\rangle =$ 0, then this would be true in a trivial way. That is, $S_z \times 0 = (b+\hbar)\times 0 = 0$. But that doesn't mean that we have succesfully used S_+ to increase the eigenvalue of S_z by $\hbar$. All we've done is annihilate our ket.

So the resolution to our dilemma must be that if you keep hitting $|a,b\rangle$ with S_+, you must eventually get 0. Let $|a,b_{\text{top}}(a)\rangle$ be the last ket we get before we reach 0. ($b_{\text{top}}(a)$ is the "top" value of b that we can reach, for this value of a.) We expect that $b_{\text{top}}(a)$ is no bigger than the square root of a. Then $S_z|a,b_{\text{top}}(a)\rangle = b_{\text{top}}(a)|a,b_{\text{top}}(a)\rangle$.

Similarly, there must exist a "bottom" state $|a,b_{\text{bot}}(a)\rangle$, such that $S_-|a,b_{\text{bot}}(a)\rangle = 0$. And $S_z|a,b_{\text{bot}}(a)\rangle = b_{\text{bot}}(a)|a,b_{\text{bot}}(a)\rangle$.

Now consider the operator $S_+S_- = (S_x+iS_y)(S_x-iS_y)$. Multiplying out the terms and using the commutation relations, we get

$S_+S_- = S_x^2+S_y^2-i(S_xS_y-S_yS_x) = S^2-S_z^2+\hbar S_z$

Hence

$$S^2 = S_+S_- + S_z^2 - \hbar S_z \tag{1}$$

Similarly

$$S^2 = S_-S_+ + S_z^2 + \hbar S_z \tag{2}$$

Now act S^2 on $|a,b_{\text{top}}(a)\rangle$ and $|a,b_{\text{bot}}(a)\rangle$:

$$\begin{aligned}
S^2|a,b_{\text{top}}(a)\rangle &= (S_-S_+ + S_z^2+\hbar S_z)|a,b_{\text{top}}(a)\rangle \\
&= (0+b_{\text{top}}(a)^2+\hbar b_{\text{top}}(a))|a,b_{\text{top}}(a)\rangle \\
S^2|a,b_{\text{top}}(a)\rangle &= b_{\text{top}}(a)(b_{\text{top}}(a)+\hbar)|a,b_{\text{top}}(a)\rangle
\end{aligned}$$

Similarly,

$$\begin{aligned}
S^2|a,b_{\text{bot}}(a)\rangle &= (S_+S_- + S_z^2-\hbar S_z)|a,b_{\text{bot}}(a)\rangle \\
&= (0+b_{\text{bot}}(a)^2-\hbar b_{\text{bot}}(a))|a,b_{\text{bot}}(a)\rangle \\
S^2|a,b_{\text{bot}}(a)\rangle &= \hbar b_{\text{bot}}(a)(b_{\text{bot}}(a)-\hbar)|a,b_{\text{bot}}(a)\rangle
\end{aligned}$$

So the first ket has S^2 eigenvalue $a = b_{\text{top}}(a)(b_{\text{top}}(a)+\hbar)$, and the second ket has S^2 eigenvalue $a = \hbar^2 b_{\text{bot}}(a)(b_{\text{bot}}(a)-\hbar)$.

But we know that the action of S_+ and S_- on $|a,b\rangle$ leaves the eigenvalue of S^2 unchanged. And we got from $|a,b_{\text{top}}(a)\rangle$ to $|a,b_{\text{bot}}(a)\rangle$ by applying the lowering operator many times. So the value of a is the same for the two kets.

Therefore $b_{\text{top}}(a)(b_{\text{top}}(a)+\hbar) = b_{\text{bot}}(a)(b_{\text{bot}}(a)-\hbar)$.

This equation has two solutions: $b_{\text{bot}}(a) = b_{\text{top}}(a)+\hbar$, and $b_{\text{bot}}(a) = -b_{\text{top}}(a)$.

But $b_{\text{bot}}(a)$ must be smaller than $b_{\text{top}}(a)$, so only the second solution works. Therefore $b_{\text{bot}}(a) = -b_{\text{top}}(a)$.

Hence b, which is the eigenvalue of S_z, ranges from $-b_{\text{top}}(a)$ to $b_{\text{top}}(a)$. Furthermore, since S_- lowers this value by $\hbar$ each time it is applied, these two values must differ by an integer multiple of $\hbar$. Therefore $b_{\text{top}}(a)-(-b_{\text{top}}(a)) = N\hbar$ for some N. So $b_{\text{top}}(a) = \frac{N}{2}\hbar$.

Hence $b_{\text{top}}(a)$ is an integer or half integer multiple of $\hbar$.

Now we'll define two variables called s and m, which will be very important in our notation later on.

Let's define $s \equiv \frac{b_{\text{top}}(a)}{\hbar}$. Then $s = \frac{N}{2}$, so s can be any integer or half integer.

And let's define $m \equiv \frac{b}{\hbar}$. Then m ranges from $-s$ to s. For instance, if $b_{\text{top}}(a) = \frac{3}{2}\hbar$, then $s = \frac{3}{2}$ and m can equal $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}$, or $\frac{3}{2}$.

Then:

$$\begin{aligned} a &= \hbar^2 s(s+1) \\ b &= \hbar m \end{aligned}$$

Since a is completely determined by s, and b is completely determined by m, we can label our kets as $|s,m\rangle$ (instead of $|a,b\rangle$) without any ambiguity. For instance, the ket $|s,m\rangle = |2,1\rangle$ is the same as the ket $|a,b\rangle = |6\hbar^2,\hbar\rangle$.

In fact, all physicists label spin kets with s and m, not with a and b. (The letters s and m are standard notation, but a and b are not.) We will use the standard $|s,m\rangle$ notation from now on.

For each value of s, there is a family of allowed values of m, as we proved. Here they are:

<u>Fact of Nature</u>: Every fundamental particle has its own special value of "s" and can have *no other*. "m" can change, but "s" does not.

If s is an integer, than the particle is a boson. (Like photons; $s = 1$)

If s is a half-integer, then the particle is a fermion. (like electrons, $s = \frac{1}{2}$)

So, which spin s is best for qubits? Spin $\frac{1}{2}$ sounds good, because it allows for two states: $m = -\frac{1}{2}$ and $\mathbf{m} = \frac{1}{2}$.

The rest of this lecture will only concern spin-$\frac{1}{2}$ particles. (That is, particles for which $s = \frac{1}{2}$).

The two possible spin states $|s,m\rangle$ are then $|\frac{1}{2},\frac{1}{2}\rangle$ and $|\frac{1}{2},-\frac{1}{2}\rangle$.

Since the s quantum number doesn't change, we only care about $m = \pm\frac{1}{2}$.

Possible labels for the two states ($m = \pm\frac{1}{2}$):

$$\begin{array}{cc} |\frac{1}{2},\frac{1}{2}\rangle & |\frac{1}{2},-\frac{1}{2}\rangle \\ |+\rangle & |-\rangle \\ |0\rangle & |1\rangle \end{array}$$

All of these labels are frequently used, but let's stick with $|0\rangle, |1\rangle$, since that's the convention in this class.

<u>Remember</u>: $|0\rangle = |\uparrow\rangle =$ state representing ang. mom. w/ z-comp. up
$|1\rangle = |\downarrow\rangle =$ state representing ang. mom. w/ z-comp. down

So we have derived the eigenvectors and eigenvalues of the spin for a spin-$\frac{1}{2}$ system, like an electron or proton:

$|0\rangle$ and $|1\rangle$ are simultaneous eigenvectors of S^2 and S_z.

$$\begin{aligned}
S^2|0\rangle &= \hbar^2 s(s+1)|0\rangle = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)|0\rangle = \frac{3}{4}\hbar^2|0\rangle \\
S^2|1\rangle &= \hbar^2 s(s+1)|1\rangle = \frac{3}{4}\hbar^2|1\rangle \\
S_z|0\rangle &= \hbar m|0\rangle = \frac{1}{2}\hbar|0\rangle, m = +\frac{1}{2} \\
S_z|1\rangle &= \hbar m|1\rangle = -\frac{1}{2}\hbar|0\rangle, m = -\frac{1}{2}
\end{aligned}$$