1 Measurement and expectation values

Last time we discussed how useful it is to work in the basis of *energy eigenstates* because of their connection with time evolution:

$$\hat{H}\psi_E = E\psi_E \Rightarrow \{\psi_E\}, \{E\}$$

Since $\hat{H}$ is a hermitian operator we know that this can be orthonormal. Time evolution is obtained by:

$$|\psi(t=0)>= a_1|\psi_{E_1}> + a_2|\psi_{E_2}> + a_3|\psi_{E_3}> + \cdots \Rightarrow |\psi(t)>= e^{-i\hat{H}t/\hbar}|\psi(t=0)>$$

So let's discuss measurement. If $|\psi>= a_1|\psi_{E_1}> + a_2|\psi_{E_2}> + a_3|\psi_{E_3}> + \cdots$, what is the result of a measurement of energy? One of the postulate of QM is that the result of the measurement must be an eigenvalue of $\hat{H}$. ψ will collapse onto one of these eigenstates with some probability. What's the probability of obtaining E_3? $P_3 = |<\psi_e|\psi>|^2 = a_3^2$ And what is ψ after measurement? ψ is projected to ψ_3 upon an observation of E_3. So, measurement is a random collapse onto one of the eig. states of the observable you are measuring!

The same holds for momentum: If we are discussing momentum then it's best to work with momentum eigenstates.

$$\hat{p}\psi_p = p\psi_p \Rightarrow \{\psi_p\}, \{p\}$$

Suppose $|\psi>= b_1|\psi_{p_1}> + b_2|\psi_{p_2}> + b_3|\psi_{p_3}> + \cdots$ What is a result of a measurement of momentum? We will end up measuring an eigenvalue of momentum with some probability, and then collapse onto that eigenstate ($P_2 = |b_2|^2$).

The exact same thing happens for the observables $\hat{x}$, $\hat{L}$, etc. The eigenstates of these observables define bases, and measurement of that observable randomly collapses us onto one of those eigenstates.

Question: What if we take an ensemble of identically prepared states and measure the same physical quantity for each? How do we determine (theoretically) the average value of the measurements? This will lead us to the definition of an *expectation value*.

Example: ENERGY. Suppose we know states $\{\psi_E\}$, $\{E\}$. If an ensemble is prepared in $|\psi>=|\psi_E>$ then the situation is simple: $<E>= E_0$. But what if we prepare an ensemble in a state $|\psi>$ in a superposition state which is not an eigenstate of $\hat{H}$, e.g. $|\psi>= a_1|\psi_{E_1}> + a_2|\psi_{E_2}> + a_3|\psi_{E_3}> + \cdots$? What is $<E>$ then?

$$<E>= E_1 Prob[E_1] + E_2 Prob[E_1] + E_3 Prob[E_3] + \cdots$$

where $Prob[E_i]$ is just

$$Prob[E_i] = | < \psi_{E_i}|\psi > |^2 = |a_i|^2$$

This yields:

$$< E >= |a_1|^2 E_1 + |a_2|^2 E_2 + |a_3|^2 E_3 + \cdots$$

Our shorthand for this is given by:

$$< E >=< \psi|\hat{H}|\psi >$$

which is known as the expectation value of the Hamiltonian (or equivalently of the energy). You can readily show that this $< E >=< \psi|\hat{H}|\psi >$ yields the proper expression.

We can do this for *any* observable! Consider arbitrary observable $\hat{A}$. The average value of this quantity for ensemble of systems prepared in $|\psi >$ is $< A >=< \psi|\hat{A}|\psi >$.

It should be noted that it is sometimes hard to evaluate the expectation value. Take the continuous basis for example ($|x >$). Suppose $\psi(x) =< x|\psi >= Ae^{-x^2}$. What is the average value of measured momentum for an ensemble of systems?

$$< \hat{p} >=< \psi|\hat{p}|\psi >= \int_{-\infty}^{\infty} \psi^*(x)\hat{p}\psi(x)dx = \int_{-\infty}^{\infty} \left(A^* e^{-x^2}\right) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \left(Ae^{-x^2}\right) dx = 0$$

So, in this instance the expectation value is zero. It is left as an exercise to evaluate $< p^2 >$ and see if *it* is zero!

2 Spin

2.1 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 docoherence and entanglement, but I'll mainly be focusing on the first three.

Examples of some possible 2-level systems are spins, atoms, photons. Others exist (such as quantum dots, superconducting loops, etc.), but I'll focus on these examples. Over the next few lectures we'll be discussing how to physically prepare, measure, and manipulate real qubit systems.

In order to manipulate qubit, we must manipulate its state:

$$|\psi>=\alpha|0>+\beta|1>$$

As you've already seen in abstract sense, this occurs by acting on $|\psi>$ with unitary operators (i.e. gates) such that

$$\hat{U}|\psi>=\alpha'|0>+\beta'|1>$$

where $\hat{U}$ is a 2×2 matrix.

2.2 The Bloch Sphere

A very nice way to think of these quantities is via the "Bloch Sphere." This is a convenient mapping for all possible single-qubit states:

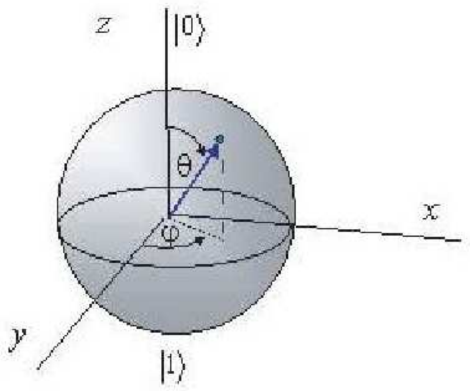


Figure 1:

θ and ϕ are the usual spherical coordinates. Every point on the sphere represents a possible qubit. All possible qubits (within an overall multiplicative phase factor) can be thought of as vectors on this unit sphere. A vector on the Bloch Sphere represents this qubit:

$$|\psi>=cos\frac{\theta}{2}|0>+e^{i\phi}sin\frac{\theta}{2}|1>$$

The action of a "gate" can be thought of as a rotation on the Bloch Sphere. Let's take the Hadamard gate **H** that has been discussed in the past. (Note that **H** is not equal to the Hamiltonian in this case!)

$$\mathbf{H}|\mathbf{0}>=\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{0}>+\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}|\mathbf{1}>$$

Given our generalized expression for a quantum state on the Bloch sphere ($|\psi>= cos\frac{\theta}{2}|0> + e^{i\phi}sin\frac{\theta}{2}|1>$), we see that the action of the Hadamard gate is to rotate the qubit by $\frac{\pi}{2}$ about the y-axis:

$$R_y\left(\frac{\pi}{2}\right)|0>= cos\frac{\pi}{4}|0> + e^{i(0)}sin\frac{\pi}{4}|0>= \frac{1}{\sqrt{2}}|0> + \frac{1}{\sqrt{2}}|1>= \mathbf{H}|\mathbf{0}>$$

But you might ask where the states $|0>$ and $|1>$ and Unitary Transformations $\hat{U}$ *actually come from*? The answer is that $|0>$ and $|1>$ are the quantum eigenstates of real systems and $\hat{U}$ arises from time evolution via the application of a Hamiltonian: $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, if $\hat{H}$ is applied for time t. The Hamiltonian transforms $|\psi>$ in the following way:

$$|\psi'>= e^{-i\hat{H}t/\hbar}|\psi>$$

So, to understand qubits we must understand the quantum levels of real physical systems and what happens to them when they are acted upon by the Hamiltonian $\hat{H}$.

The first physical quantum system that we will investigate is *SPIN*. We will spend a bunch of time on spin, since all other qubit systems can be mapped onto an effective spin system.

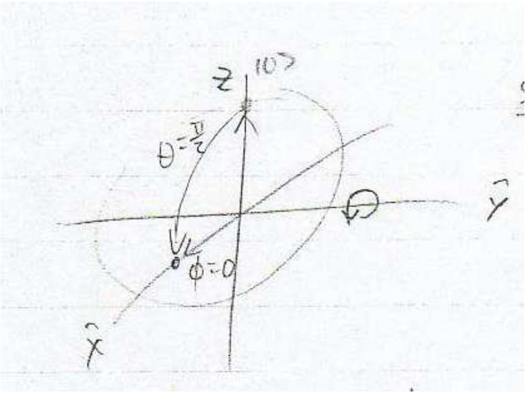
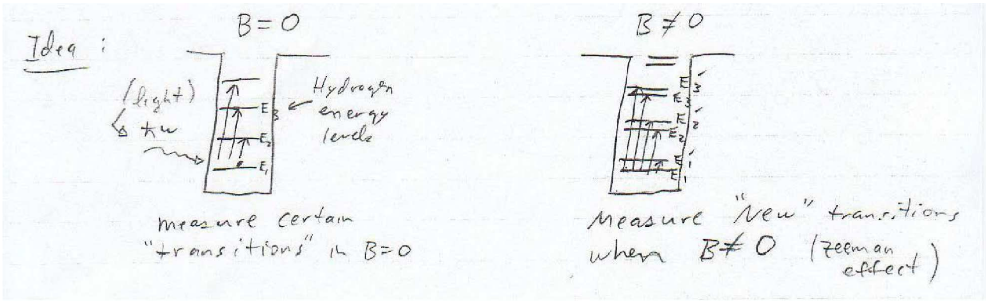


Figure 2:

2.3 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. The 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 $|\uparrow>= |0>$, $|\downarrow>= |1>$.

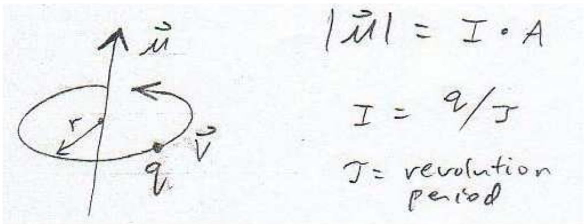
How do we understand the details of spin? The history of the development of spin is an interesting one. The ”discovery” of spin is largely credited to Uhlenbeck and Gondsmit who, in 1925, introduced it to explain the behavior of hydrogen atoms in a magnetic field:



This can be explained if an electron has an *intrinsic* magnetic moment $\vec{\mu}$ since a magnetic moment in a magnetic field $\vec{B}$ has an energy $E = -\vec{\mu} \cdot \vec{B}$. In the context of QM, new energy levels come from $\vec{\mu}$ either parallel or anti-parallel to $\vec{B}$.

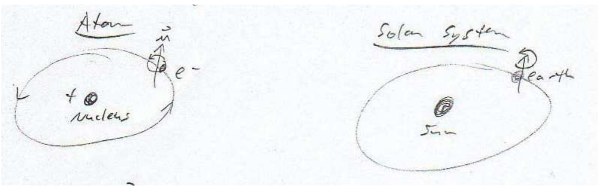
But where does $\vec{\mu}$ come from, and how do we explain its QM behavior?

The simplest explanation is “Classical”: Classically, $\vec{\mu}$ comes from a loop of current.



The energy $E = -\vec{\mu} \cdot \vec{B}$ comes from $\vec{I} \times \vec{B}$ force of current in a B-field (Lorentz force). The lowest energy, and thereby the place where ”the system wants to go”, is obtained when the magnetic moment and B-field line up.

If an isolated electron has “intrinsic” $\vec{\mu}$ then the simplest explanation for this is that electron spins about some axis. this is independent of orbital motion in atom, just like the Earth’s ”spin” about the north pole is independent of its orbit around sun.



Since $\vec{\mu}$ is associated with “spinning” charge, then we can write $\vec{\mu}$ in terms of angular momentum. Anything that spins has angular momentum!

The simplest way to see this is classically for a spinning charge. Angular momentum is given by $\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times m\vec{v}$. $L = mvr$ for a charge of mass $= m$ moving in a a circle with velocity $= v$. The magnetic moment can be obtained as follows:

$$\mu = (current)\,(Area) = \frac{e}{J} \cdot \pi r^2$$

But $I = \frac{2\pi r}{v}$, so

$$\mu = \frac{e}{2} \cdot vr = \frac{e}{2} \cdot \frac{L}{m} \Rightarrow \vec{\mu} = -\frac{e}{2m}\vec{L}$$

Now comes the tricky part. *The electron is not actually spinning about some axis!* It only acts as though it is. Electrons are point particles which, as far as we know, have no "size" in the traditional sense. Therefore the r in the previous discussion of spinning charge is not meaningful. The *intrinsic* angular momentum of an electron has nothing to do with "orbital" motion, but it does lead to an intrinsic $\vec{\mu}$. This 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.

This intrinsic angular momentum is called "spin" = $\vec{S}$.

Classically: $\vec{\mu} = -\frac{e}{2m}\vec{L}$

Quantum Mechanically: $\vec{\mu} = -\frac{ge}{2m}\vec{S}$

What is g? g is called the g-factor and it is a unitless correction factor due to QM. 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 $\mu_{\vec{proton}} \ll \mu_{\vec{electron}}$.

So, to understand behavior of electron's intrinsic magnetic moment $\vec{\mu}$ (which is an observable we can measure) then we must understand the behavior of its intrinsic angular momentum = $\vec{S}$. This is why spin is important. Since the electron is small, $\vec{S}$ must be described by QM.

To understand spin = $\vec{S}$ we must first understand the QM properties of angular momentum. Classically, angular momentum is $\vec{L} = \vec{r} \times \vec{p} = \hat{L}_x\mathbf{i} + \hat{\mathbf{L}}_\mathbf{y}\mathbf{j} + \hat{\mathbf{L}}_\mathbf{z}\mathbf{k}$ 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 any general properties we derive for the QM operator $\vec{L} = \vec{r} \times \vec{p} = \hat{L}_x\mathbf{i} + \hat{\mathbf{L}}_\mathbf{y}\mathbf{j} + \hat{\mathbf{L}}_\mathbf{z}\mathbf{k}$ we can simply apply to the operator $\vec{S} = \vec{S}_x\mathbf{i} + \tilde{\mathbf{S}}_\mathbf{y}\mathbf{j} + \tilde{\mathbf{S}}_\mathbf{z}\mathbf{k}$. This is the standard treatment.

Now I will quote some properties that are straightforward to derive for $\vec{L} = \vec{r} \times \hat{P}$, and I will apply them directly to the operator $\vec{S}$. (I will skip the derivations, but they are done in standard texts and will be left as HW assignment.)

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 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 $\hat{S}_y|s_x, s_y> = s_y|s_x, s_y>$.

Kind of a bummer. 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 only one component of $\vec{S}$. Following standard convention, let's pick $S_i = S_z$. We can find spin states $|s,m>$ that are simultaneous eigenstates of $\vec{S}^2$ and $\hat{S}_z$.

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

To understand "spin", we must understand spin eigenstates $|s,m>$. First, what are allowed values of a_s, b_m? These are eigenvalues of operators representing observables. Obviously this is very important since they are what you measure! We'll explore these eigenvalues and eigenstates in the next lecture.