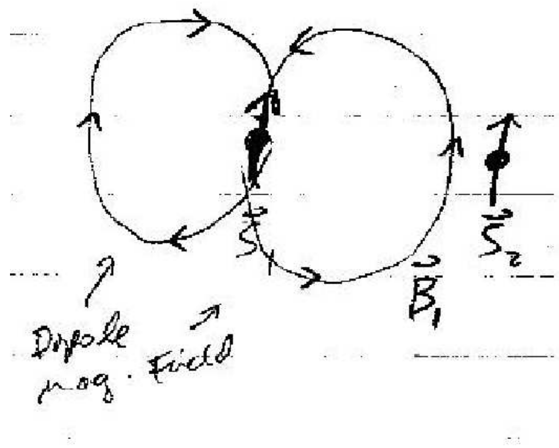
1 Entanglement and Spin

So far we've talked about 1 qubit operations (e.g. $|\psi\rangle \Rightarrow |\psi'\rangle = \alpha'|0\rangle + \beta'|1\rangle$). But what about entanglement? What about when there are more than one qubits?

Question: How do we physically create an entangled state of 2 spins?

Answer: Must have an interaction between them, i.e. *two* particle Hamiltonian.

How do we create such an interaction and how does it lead to entanglement? Let's start with two physical qubits, say, electrons:



Claim: The ground state of this system is an entangled state! Namely, $|\psi\rangle = \frac{1}{2}\left(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2\right)$, a Bell state!

How do we show this? It's the same old quantum story, solving the Schr. equation.

So what is $\hat{H}$? We must figure out how these electrons interact with each other. What effect could one electron have on the other electron, and vice versa?

Well, we know that an electron has a magnetic dipole moment that is related to its spin. Magnetic dipole moments come up classically when you have current loops, so conceptually we can think of electrons as little current loops that generate dipolar magnetic fields. But if one electron generates a magnetic field, then the other electron can "feel" that electric field. If you put two electrons close enough together, then we imagine that the two generated fields from electron #1 (#2) will be felt by electron #2 (#1).

What does this look like mathematically, i.e. what is the Hamiltonian? Well, we know $\vec{\mu} = -\frac{e}{m}\vec{S}$ and $\hat{H} = \vec{\mu} \cdot \vec{B}$. But we know that the magnetic field produced by a magnetic moment is proportional to that vector, so we can say $\vec{B}_1 \propto \vec{S}_1$, or $\vec{B}_1 = A\vec{S}_1$ where $A > 0$. So,

$$\hat{H} = -\left(-\frac{e}{m}\vec{S}_2\right) \cdot A\vec{S}_1 \tag{1}$$

or equivalently,

$$\hat{H} = C\vec{S}_2 \cdot \vec{S}_1 \tag{2}$$

where $C > 0$. This is our electron interaction Hamiltonian. You might wonder what C is. C should be a strong function of the relative position, but we don't want to worry about that now. You can just imagine that C is determined through experiment, but is equal to some value that is yet to be determined. The important part is the $\vec{S}_1 \cdot \vec{S}_2$ term.

So what is the ground state of this Hamiltonian? Let's use a little trick (whenever you hear "trick" in regards to spins and angular momentum, it's time to bust out the raising/lowering operators).

Consider $\vec{S}_{Total} = \vec{S}_1 + \vec{S}_2$, a new operator that should represent the *total* spin of the two electron system. Let's look at some features of this new operator:

$$\vec{S}_T \cdot \vec{S}_T = \hat{S}_T^2 = \left(\vec{S}_1 + \vec{S}_2\right) \cdot \left(\vec{S}_1 + \vec{S}_2\right) = \hat{S}_1^2 + \hat{S}_2^2 + 2\vec{S}_2 \cdot \vec{S}_1 \tag{3}$$

We see that the dot product $\vec{S}_2 \cdot \vec{S}_1$ has appeared. Let's solve for this quantity:

$$\vec{S}_2 \cdot \vec{S}_1 = \frac{1}{2}\left(\hat{S}_T^2 - \hat{S}_1^2 + \hat{S}_2^2\right) \tag{4}$$

and therefore our interaction Hamiltonian can be expressed as:

$$\hat{H} = \frac{C}{2}\left(\hat{S}_T^2 - \hat{S}_1^2 + \hat{S}_2^2\right) \tag{5}$$

So, the ground state will be whatever state minimizes the expectation value of this operator (recall $< E >= \left\langle\psi\middle|\hat{H}\middle|\psi\right\rangle$).

Note that no matter what $\left|\psi\right\rangle$ is, $\hat{S}_1^2\left|\psi\right\rangle = \hbar^2\frac{1}{2}\left(\frac{1}{2}+1\right)\left|\psi\right\rangle = \frac{3}{4}\hbar^2\left|\psi\right\rangle$. The same goes for $\hat{S}_2^2$, so we can replace both $\hat{S}_1^2$ and $\hat{S}_2^2$ with $\frac{3}{4}\hbar^2$. We see that the Hamiltonian can be rewritten as:

$$\hat{H} = D\hat{S}_T^2 - F \tag{6}$$

where D and F are constants greater than zero. So what state $\left|\psi\right\rangle$ has the smallest $\left\langle\psi\middle|\hat{S}_T^2\middle|\psi\right\rangle$? The best we could hope for is $\left|\psi\right\rangle$ such that $\left\langle\psi\middle|\hat{S}_T^2\middle|\psi\right\rangle = 0$.

It is left to a homework problem to show that the following state

$$\left|\psi\right\rangle_o = \frac{1}{\sqrt{2}}\left(\left|0\right\rangle_1\left|1\right\rangle_2 - \left|1\right\rangle_1\left|0\right\rangle_2\right) \tag{7}$$

is an eigenstate of $\hat{S}_T^2$ with eigenvalue 0.

We conclude from this that we can experimentally create a Bell state by putting 2 spins next to each other and then providing a perturbation such that the fall into the ground state!

2 Interaction Hamiltonians in General

Electron spins are hardly the only quantum system that can be entangled, so we might want to talk about general entanglement through "interaction Hamiltonians." In the most general sense, we can talk about two quantum numbers x_1 and x_2 (i.e. quantized physical observables) that yield the following Hamiltonian:

$$\hat{H}(x_1, x_2) = \hat{H}_1(x_1) + \hat{H}_2(x_2) + \hat{H}'(x_1, x_2) \tag{8}$$

where $\hat{H}'(x_1, x_2) \neq \hat{H}_1'(x_1) + \hat{H}_2'(x_2)$. If this is the case, then resultant energy eigenstates will not in general be product states:

$$\psi(x_1, x_2) \neq \psi_1(x_1) \cdot \psi_2(x_2) \tag{9}$$

This is the definition of entanglement! Therefore, in our quest for entanglement we need to focus our attention on interaction Hamiltonians. In the case of spins, $\hat{H} = C\hat{S}_1 \cdot \hat{S}_2$ is such a Hamiltonian, and we will explore others in coming lectures.

3 Introduction to Atomic Qubits

Whenever we think of qubits we will try to draw analogies to the spin-1/2 system, but let's now consider another very useful quantum system: Atoms!

What is an atom? How can it be thought of as a qubit?

Quick answer: An atom is a tiny box that holds electrons in discrete energy levels. If I can focus on one particular electron that can hop between 2 different states, then that is a qubit!

Question: How do we measure and manipulate this qubit? Equivalently, how do we control $\left|\psi\right\rangle$, the state of the valence electron?

Answer: Apply a Hamiltonian!! Apply an external field that leads to some $\hat{H}$ (to quote Dr. Evil, this is usually done with a "laser").

Once we've created the desired Hamiltonian, as usual we solve the Schr. Equation (is this sounding like a broken record yet?). The Hamiltonian drives the time development of the system through the time development operator $e^{-i\hat{H}t/\hbar}$ and we can change $\left|\psi\right\rangle \rightarrow \left|\psi'\right\rangle$.

Note: if we keep our focus on only one electron hopping between two states then this problem is *identical* to the spin-1/2 problem! We have to relabel some quantities, but the physics (and ultimately the results) are the same. Our atomic state (specified by the state of the valence electron) $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ can be thought of as a vector on the Bloch sphere, even though it's not spin.

To move forward, however, we must have a better idea of $|0\rangle$ and $|1\rangle$ actually are, and how do we compute $\hat{H}$ and its action on $|\psi\rangle$. $|0\rangle$ and $|1\rangle$ are atomic energy levels for a single atom. Equivalently we could say that $|0\rangle$ and $|1\rangle$ are the energy eigenstates for an electron orbiting a nucleus.

$$\begin{aligned} \hat{H}_o|0\rangle &= E_o|0\rangle \\ \hat{H}_o|1\rangle &= E_1|1\rangle \end{aligned} \tag{10}$$

So what is the Hamiltonian $\hat{H}_o$ describing this? We can focus on hydrogen because it's conceptually simple. Practically, experimentalists don't usually work with hydrogen because it's pretty tricky to deal with. A large chunk of modern atomic physics (esp. quantum computing research!) is done with hydrogenic atoms (i.e. alkali metals and ions with a single valence electron).

Anyway, what is $\hat{H}_o$ for the simplest atom, hydrogen? $\hat{H}_o$ comes from classical energy:

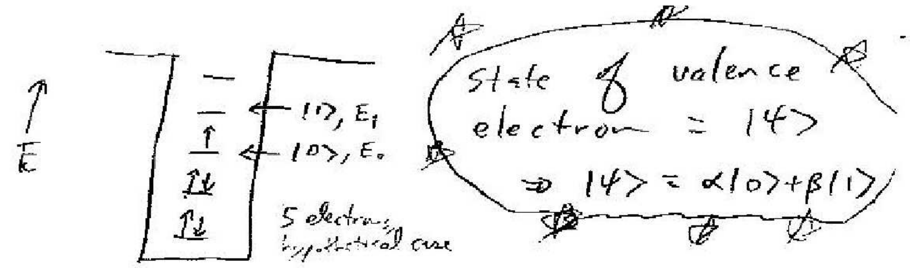
$$\begin{aligned} E &= KE + PE \\ E &= \tfrac{p^2}{2m} + \tfrac{-e^2}{r} \end{aligned} \tag{11}$$

So, in the quantum mechanical way, we turn classical observables like position and momentum into operators, and this gives us our hydrogenic Hamiltonian:

$$\hat{H}_o = \tfrac{\hat{p}^2}{2m} + \tfrac{-e^2}{|\hat{r}|} \tag{12}$$

To get the energy levels of hydrogen we just need to solve this Hamiltonian. This would be large aside for this course, so if you're interested (and you should be!) then you should take a QM course like 137A.

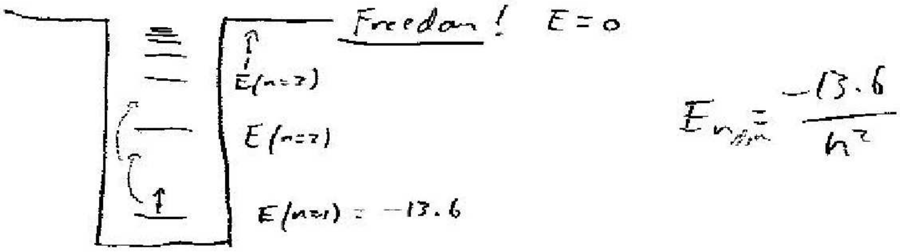
You can take it as given that this Hamiltonian yields quantized energy levels and nice, pretty-looking wavefunctions. Let's take a look at the general form of these wavefunctions (expressed in the natural coordinate



system, spherical coordinates):

$$\psi_n(\vec{r}) = \psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\,Y_{lm}(\theta,\phi)$$
$$E_{nlm} = \frac{-13.6eV}{n^2} \tag{13}$$

So we get electronic wavefunctions in three dimensions with three quantum numbers: n, l, and m. n is called the principle quantum number, since it determines the energy. l is the magnitude of the orbital angular momentum, it being the eigenvalue index of the $\hat{L}^2$ operator (this is exactly equivalent to s being the index of the $\hat{S}^2$ operator, except that l can only take on integer values). m is the eigenvalue index of $\hat{L}_z$ (again, just like m for $\hat{S}_z$.



The energy levels can be degenerate (many quantum states at the same energy), and some degeneracies can be lifted by various perturbations. We are going to ignore all this detail, which again would be covered *ad nauseum* in a course like 137A.

Even though the hydrogenic Hamiltonian has resulted in a infinite number of possible states, we can assume that the electron spends most of its time hopping between just two states and ignore the others. This is a surprisingly good approximation!

$|0\rangle \rightarrow R_{nl}(r)\,Y_{lm}(\theta,\phi)$ for some n, l, m; $E_o = E_{n,l,m}$

$|1\rangle \rightarrow R_{n'l'}(r)\,Y_{l'm'}(\theta,\phi)$ for some n', l', m'; $E_1 = E_{n',l',m'}$

Okay, now we know what $|0\rangle$ and $|1\rangle$ look like. What does $\hat{H}$ look like in the restricted subspace defined by $|0\rangle$ and $|1\rangle$?

This is a slightly awkward question, since I already told you for an "unperturbed" atom $\hat{H} = \hat{H}_o = \frac{\hat{p}^2}{2m} + \frac{-e^2}{|\hat{r}|}$. So, you might say that "$\hat{H}$ is a function of position, $\vec{r}$." Or, you might say that "$\hat{H}$ is a 2×2 matrix."

Both of these answers are correct! How do we reconcile them? KEY POINT: $\hat{H}$ looks different for different bases!!

If we're talking about the motion of an electron through space around the nucleus, then a convenient basis is $\{|\vec{r}\rangle\}$, the set of all points $\vec{r}$ throughout space. In this case, $\hat{H} = f(\vec{r})$, a function of $\vec{r} \Rightarrow$ could construct a matrix using $H_{r_1,r_2} = \langle \vec{r}_1|\hat{H}|\vec{r}_2\rangle$ ... but let's not!

If we're talking about jumps between two quantum levels, $|0\rangle$ and $|1\rangle$, then a convenient basis is $\{|0\rangle, |1\rangle\}$. This is a 2-D basis, so $\hat{H}$ is a 2×2 matrix:

$$\hat{H}_o \rightarrow \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \tag{14}$$

The moral of the story is to choose your basis wisely!

How do we construct the matrix H_{ij}? We must find the matrix elements $\langle i|\hat{H}_o|j\rangle$:

$$
\begin{aligned}
H_{11} &= \langle 0|\hat{H}_o|0\rangle = E_o\langle 0|0\rangle = E_o \\
H_{12} &= \langle 0|\hat{H}_o|1\rangle = E_1\langle 0|1\rangle = 0 \\
H_{21} &= \langle 1|\hat{H}_o|0\rangle = E_o\langle 1|0\rangle = 0 \\
H_{22} &= \langle 1|\hat{H}_o|1\rangle = E_1\langle 1|1\rangle = E_1
\end{aligned}
\tag{15}
$$

So our matrix becomes:

$$
\hat{H}_o \rightarrow \begin{pmatrix} E_o & 0 \\ 0 & E_1 \end{pmatrix} \tag{16}
$$

So, we now have the Hamiltonian that describes the state of an electron in an unperturbed atom. Note that this looks just like the Hamiltonian for a spin in a magnetic field! $\hat{H} \rightarrow \frac{e\hbar}{2m}\begin{pmatrix} B_o & 0 \\ 0 & -B_o \end{pmatrix}$

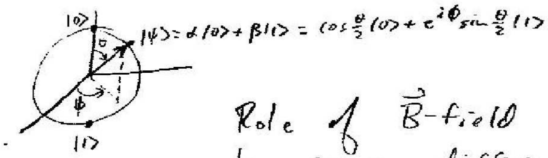
Let's use this Hamiltonian to get some time-dependence going:

$$
|\psi(t=0)\rangle = \alpha|0\rangle + \beta|1\rangle \Rightarrow |\psi(t)\rangle = e^{-i\hat{H}_o t/\hbar}|\psi(0)\rangle \tag{17}
$$

So, we get the following time dependent state:

$$
|\psi(t)\rangle = \alpha|0\rangle e^{-iE_o t/\hbar} + \beta|1\rangle e^{-iE_1 t/\hbar} \tag{18}
$$

Geometrically, this can be interpreted as a vector on the Bloch sphere, just like for spin (even though it's not actually spin).



Role of $\vec{B}$-field ($B_o\hat{z}$) is now played by energy difference $E_1 - E_o$

If $|\psi(0)\rangle$ starts off at (θ_o, ϕ_o), at a time t later $|\psi(t)\rangle$ has rotated by $\Delta\phi$ around the $\hat{z}$ axis at angular frequency $\omega_o = \frac{E_1 - E_2}{\hbar}$.

BUT, we see that $\hat{H}$ will never induce "spin-flips," i.e. change ratio between $|0\rangle$ and $|1\rangle$ (i.e. change θ). How do we do *that*? We'll see next lecture...