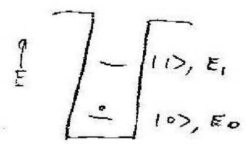
1 Atomic Qubits

Consider an atom where only 2 atomic states are important:



$\Rightarrow H_o|1\rangle = E_1|1\rangle$

$H_o|0\rangle = E_o|0\rangle$

|0>, |1> refer to atomic orbitals

$|0\rangle$, $|1\rangle$ refer to atomic orbitals:

$$|0\rangle, |1\rangle \rightarrow \psi_{nlm}(r,\theta,\phi)|s,m_s\rangle = R_{nl}(r)Y_{lm}(\theta,\phi)|s,m_s\rangle$$

Atomic wave function can be quite complex, but let's not worry about this detail (can be looked up in any number of books). We'll just assume it exists.

What does $\hat{H}_o$ look like in the basis of $|0\rangle$, $|1\rangle$? We showed before that it looks like $\hat{H}_o = \begin{pmatrix} E_o & 0 \\ 0 & E_1 \end{pmatrix}$. Note that the energy difference $(E_1 - E_o)$ plays the same role as B_o did for spin!

Now consider an arbitrary electronic state: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. How does it change in time? $|\psi(t)\rangle = e^{-i\hat{H}_o t/\hbar}|\psi\rangle = \alpha e^{-iE_o t/\hbar}|0\rangle + \beta e^{-iE_1 t/\hbar}$.

We can project this onto the Bloch sphere (just like spin!): $|\psi(t)\rangle \rightarrow \alpha|0\rangle + \beta e^{-i(E_1-E_o)t/\hbar}|1\rangle$.

We immediately see that the state vector spins around the z-axis with $\omega_o = \frac{E_1-E_o}{\hbar}$. *But*, although $\hat{H}_o$ causes $|\psi(t)\rangle$ to spin around the z-axis, it will never cause it to change "latitude" on the Bloch sphere. This means that that for the unperturbed Hamiltonian, there are no spin flips or transitions... how can we accomplish *this*?

Question: How do we change our atomic qubit state in a way that θ changes where $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = cos\frac{\theta}{2}|0\rangle + e^{i\phi} sin\frac{theta}{2}|1\rangle$?

Answer: Need to perturb our system with a "Force Field" so that the Hamiltonian gets off-diagonal elements!!

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

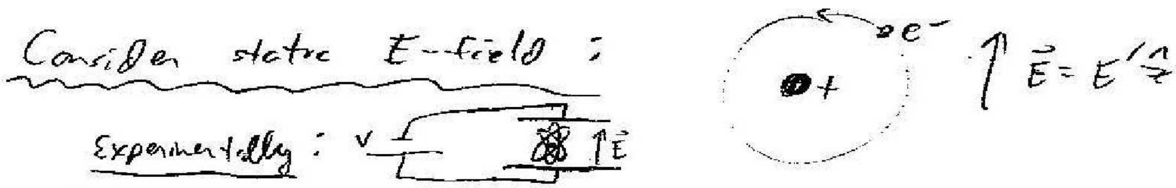
In order to change ratio between occupancy of $|0\rangle$ and $|1\rangle$ we must have $H_{12} \neq 0$. There are no off-diagonal terms in $\hat{H}_o$, so we need a new term in the Hamiltonian.

How do we get a new term? One natural way would be turn on an external electric field. This applies a force that causes $H_{12} \neq 0$ and induces "vertical" rotations on Bloch sphere in exactly the same manner as $\vec{B}$ did for spin. To understand this, we must understand what happens when we subject an atom to an $\vec{E}$-field. How do we do this? Solve the Schrodinger equation, of course.

First off, we need to find the perturbing Hamiltonian. That is, the electric field contributes to the energy of the system, and this must be accounted for in our overall Hamiltonian.

So what is the classical energy of an atom in an $\vec{E}$-field? We must find the energy of this "perturbation."

Let's first consider a static E-field:



Only worry about the electron, since it is much lighter than nucleus.

$$\vec{F} = -e\vec{E} = -eE'\hat{z}$$

$$energy = U = -\int \vec{F} \cdot d\vec{r}$$

$$U = -\int -eE'\hat{z} \cdot d\vec{r} = \int eE'dz = eE'z$$

So the potential energy depends on z-location of electron. This is the energy term that causes transitions between $|0\rangle$ and $|1\rangle$!! Our complete Hamiltonian is now $\hat{H} = \hat{H}_o + \hat{H}'$, where $\hat{H}' = eE'z$. The "z" in the last term is actually the z-operator, but the hat might get confused with the unit vector so we drop it here. (Incidentally, the British have a handy way to denote vectors which alleviate this hat-vector-operator confusion. They express vectors by underlining variables with tilde's ( )... too bad we're not British.)

$\hat{H}'$ is called the "dipole" Hamiltonian since if we define an electric dipole $\vec{p} = -e\vec{r}$. (Another unfortunate variable confusion... this is certainly NOT momentum!)

$$\hat{H}' = -\vec{p} \cdot \vec{E} = -(-e\vec{r}) \cdot E'\hat{z} = eE'z$$

So how does $\hat{H}'$ change the 2×2 representation of $\hat{H}$, and how can this be used to control $|\psi\rangle$?

To see how qubit changes under influence of perturbation we must find $\hat{H}$ and solve the time-dependent Schrodinger equation. Again, we express the Hamiltonian as a matrix:

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

It is our job to now calculate these matrix elements H_{ij}. Let's start with H_{11}:

$$H_{11} = \left\langle 0 \right| \left(\hat{H}_o + eE'z\right) \left|0\right\rangle = \left\langle 0 \middle| \hat{H}_o \middle| 0 \right\rangle + \left\langle 0 \middle| eE'z \middle| 0 \right\rangle = E_o + \left\langle 0 \middle| eE'z \middle| 0 \right\rangle$$

So let's find $\left\langle 0 \middle| eE'z \middle| 0 \right\rangle$. This is most easily accomplished in spherical coordinates:

$$\left\langle 0 \middle| eE'z \middle| 0 \right\rangle = \int_r \int_\theta \int_\phi R^*_{nl}(r) Y^*_{lm}(\theta,\phi) \left(eE'rcos\theta\right) R_n l(r) Y_{lm}(\theta,\phi) r^2 sin\theta dr d\theta d\phi$$

As it turns out, this integral is zero. There is an electric dipole selection rule that states that $\Delta l = \pm 1$ for the angular integral to be nonzero. In this case $\Delta l = 0$, so the whole above integral is zero. This means that $H_{11} = E_o$. Similarly, $\left\langle 1 \middle| eE'z \middle| 1 \right\rangle = 0$ so $H_{22} = E_1$.

But what about the crucial H_{12} ($= H^*_{21}$) term?

$$H_{12} = \left\langle 0 \right| \left(\hat{H}_0 + eE'z\right) \left|1\right\rangle = \left\langle 0 \middle| \hat{H}_o \middle| 1 \right\rangle + \left\langle 0 \middle| eE'z \middle| 1 \right\rangle$$

but $\left\langle 0 \middle| \hat{H}_o \middle| 0 \right\rangle = E_1 \left\langle 0 \middle| 1 \right\rangle = 0$. So we're left with finding $\left\langle 0 \middle| eE'z \middle| 1 \right\rangle$... to do this, we need to calculate this integral:

$$\left\langle 0 \middle| eE'z \middle| 1 \right\rangle = \int_r \int_\theta \int_\phi R^*_{nl}(r) Y^*_{lm}(\theta,\phi) \left(eE'rcos\theta\right) R_n l(r) Y_{lm}(\theta,\phi) r^2 sin\theta dr d\theta d\phi$$

Because $\left|0\right\rangle \neq \left|1\right\rangle$ they may have different l and the states may be chosen such that $\Delta l = l' - l = \pm 1$ so that the above integral has a nonzero value.

Assume the integral is known, and we can define $V_1 = \left\langle 0 \middle| eE'z \middle| 1 \right\rangle$. Since $\hat{H}$ is Hermitian, we know that $H_{21} = V_1^*$. So, we write down our Hamiltonian matrix:

$$\hat{H} \rightarrow \begin{pmatrix} E_o & V_1 \\ V_1^* & E_1 \end{pmatrix}$$

We immediately see that the off-diagonal matrix elements are nonzero and we can induce transitions between $\left|0\right\rangle$ and $\left|1\right\rangle$! What does this look like geometrically on the Bloch sphere? Here we use the analogy to spin.

The energy difference plays the role of $\vec{B} = B_o \hat{z}$. The applied $\vec{E}$-field plays the role of the perpendicular magnetic field $\vec{B}_1$. The off-diagonal matrix element V_1 plays the role of $\vec{B}_1 = B_x \hat{x}$. What happens? $B_x = V_1$ causes total $\vec{B}$-field to "tilt," and $\left|\psi\right\rangle$ rotates around new total $\vec{B}$-field:

So, the latitude on Bloch sphere does change, i.e. " θ" will NOT change by much unless $\vec{B}_x \approx \vec{B}_o$. In other words, for a significant change in θ we need $V_1 \approx E_1 - E_o$.

Unfortunately this is easier said than done in the case of atoms. It would require fields on the order of Volts/Angstrom, since the size of an atom is about 1 Angstrom and $E_1 - E_o \approx 1eV$. The capacitor plates would need to be extremely close, and this is unreasonable.

So, what else can we do to control the state of our electronic qubit? How can we change "θ"?

Answer: Use resonance technique, which is exactly what we did for spin resonance!

Oscillate the $\vec{E}$-field at the frequency $\omega_o = \frac{E_1 - E_o}{\hbar}$... this allows us to control $\theta(t)$ very precisely. So, let's modify our static electric field to be oscillatory:

$$\vec{E}' \rightarrow E' cos \omega_o t \hat{z}$$

It is important to note that the frequency ω_o is very large! $E_1 - E_o \approx eV \Rightarrow \omega_o \approx 10^{15} Hz$. That's the frequency of light!

So, to create $\vec{E} = E' cos \omega_o t \hat{z}$, we don't use a capacitor plate but instead we shine light on the atom!! Light is exactly the oscillatory field we need.

So, what does an atomic qubit do when we shine light on it? We must solve the Schr. equation: $i\hbar \frac{\partial}{\partial t} \left|\psi\right\rangle = \hat{H} \left|\psi\right\rangle$

$$\hat{H} \rightarrow \begin{pmatrix} E_o & V_1 cos \omega_o t \\ V_1^* cos \omega_o t & E_1 \end{pmatrix}$$

This is essentially the same problem that we solved before for an oscillating $\vec{B}$ applied to spin. Before we found that $\left|\psi(t)\right\rangle = cos \frac{\omega_1 t}{2} \left|0\right\rangle + e^{i(\omega_o t + \pi)} sin \frac{\omega_1 t}{2} \left|1\right\rangle$ where $\omega_o \propto B_o$, $\omega_1 \propto B_1$.

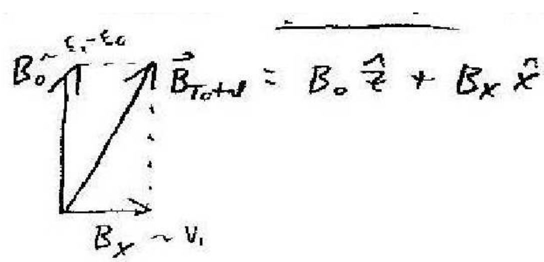
Now we can map our atomic system onto the spin problem and we see that $\omega_o = \frac{E_1 - E_o}{\hbar}$ (the qubit energy splitting) and $\omega_1 = \frac{V_1}{\hbar}$ (the intensity of light at ω_o shined on the qubit. $\left|\psi\right\rangle$ now changes latitude on Bloch sphere at rate $\omega_1 = \frac{V_1}{2\hbar}$.

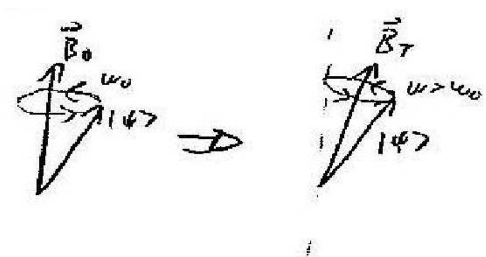
OK, so now we see that we can control $\left|\psi\right\rangle = \alpha \left|0\right\rangle + \beta \left|1\right\rangle = cos \frac{\theta}{2} \left|0\right\rangle + e^{i\phi} sin \frac{\theta}{2} \left|1\right\rangle$ very precisely by shining well-timed pulses of light at the atomic qubit. Suppose we put atom into such an arbitrary state. How do we measure α and β?

One attractive answer is fluoresence. What we can do is pick atom that has a third state $\left|2\right\rangle$ that couples to $\left|1\right\rangle$ but NOT to $\left|0\right\rangle$!!

You might wonder how this would work. We stated before that dipole transitions require $\Delta l = \pm 1$. We could make our three state system as follows: $\left|0\right\rangle = \left|l = 0\right\rangle$, $\left|1\right\rangle = \left|l = 1\right\rangle$, and $\left|2\right\rangle = \left|l = 2\right\rangle$. We can immediately see that we'll get transitions from $\left|0\right\rangle \rightarrow \left|1\right\rangle$ and $\left|1\right\rangle \rightarrow \left|2\right\rangle$, but no transitions from $\left|0\right\rangle \rightarrow \left|2\right\rangle$!

So, if we want to measure whether the atom is in either state $\left|0\right\rangle$ or $\left|1\right\rangle$, we can just shine light on the atom of frequency $\frac{E_2 - E_1}{\hbar}$. If the atom is in state $\left|0\right\rangle$, then nothing happens. But, if the atom is in the state $\left|1\right\rangle$ then the electron will absorb a photon and get pushed up to state $\left|2\right\rangle$. The electron will then tend to fall back down the energy ladder and re-radiate the photon. *This can be detected!*





This is just like Stern-Gerlach, in the sense that we get a different signal if electron is in the state $\left|0\right\rangle$ and $\left|1\right\rangle$. Our recipe for measuring $|\alpha|$ and $|\beta|$: we prepare an atom in the state $\left|\psi\right\rangle = \alpha\left|0\right\rangle + \beta\left|1\right\rangle$ and then shine light on it and see if it absorbed a photon. Then we prepare the state again and repeat the experiment. Suppose you do this 1000 times and it absorbs the photon 800 times. What is β?

$$|\beta|^2 = probability = \frac{800}{1000} = \frac{8}{10} \Rightarrow |\beta| = \sqrt{\frac{8}{10}}, |\alpha| = \sqrt{\frac{2}{10}}$$

But what about the relative phase between α and β? This is more difficult, because we have to rotate $\left|\psi\right\rangle$ by 90^o around $\hat{y}$ and measure $< S_z >$ to get $< S_x >$. Similarly we need $< S_y >$ because $< S_x >$ and $< S_y >$ define ϕ. Tricky, but doable...