Cheng O.H. 9-10, to later !!

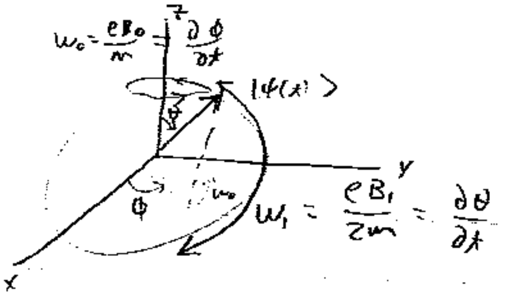
spin-spin entanglement
Atoms as qubits
(electronic levels)
midterm

10/9/03 (1)

Crommie Lecture #6

<u>Last time</u>: Talked about spin resonance, turn on AC B-field $\perp$ to DC field $\Rightarrow$ get off-diag. matrix elements in Hamiltonian

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \frac{e\hbar}{2m} \begin{pmatrix} B_0 & B_1 \cos\omega_0 t \\ B_1 \cos\omega_0 t & -B_0 \end{pmatrix}$$



Also talked about how one can get entanglement between 2 spins $\Rightarrow$ Need interaction between them!

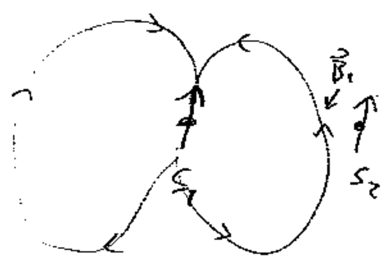
<u>Need</u> $H(x_1, x_2) = H_1(x_1) + H_2(x_2) + H'(x_1, x_2)$

where $H'(x_1, x_2) \neq H_1'(x_1) + H_2'(x_2)$

$\Rightarrow \psi(x_1, x_2) \neq \psi_1(x_1) \cdot \psi_2(x_2)$, defn of entanglement!

<u>For 2 stationary spins</u>: Interaction is due to fact that one spin feels $\vec{B}$-field of the other spin:

Dipole field



[Like Hyperfine splitting]

$\vec{S}_2$ "feels" $\vec{B}_1$ due to $\vec{S}_1$

$\Rightarrow \hat{H} = -\vec{\mu}_2 \cdot \vec{B}_1$, $\quad \vec{B}_1 \propto \vec{S}_1$, $\quad \vec{\mu}_2 \propto \vec{S}_2$

$\therefore \hat{H} = C\,\vec{S}_2 \cdot \vec{S}_1$ where $C > 0$

$\Rightarrow H \neq H_1 + H_2 \Rightarrow$ causes entanglement

Claim: g-state of this Hamiltonian is an entangled state! A Bell state!

How do we show this? Must find g-state of $\hat{H} = C\,\vec{S}_1 \cdot \vec{S}_2$!

Do a little trick: Consider $\vec{S}_{Total} = \vec{S}_1 + \vec{S}_2$ {A new operator!

$\Rightarrow \vec{S}_T \cdot \vec{S}_T = S_T^2 = (\vec{S}_1 + \vec{S}_2)\cdot(\vec{S}_1 + \vec{S}_2) = S_1^2 + S_2^2 + 2\,\vec{S}_2 \cdot \vec{S}_1$

$\Rightarrow \vec{S}_2 \cdot \vec{S}_1 = \frac{1}{2}\left(S_T^2 - S_1^2 - S_2^2\right)$

$\Rightarrow \boxed{\hat{H} = \frac{C}{2}\left(\hat{S}_T^2 - \hat{S}_1^2 - \hat{S}_2^2\right)}$ ← So, g-state is whatever state minimizes expectation value of this operator.

$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle$

Note: No matter what $|\psi\rangle$ is, $\hat{S}_1^2 |\psi\rangle = \hbar^2 \frac{1}{2}(\frac{1}{2}+1)|\psi\rangle = \frac{3}{4}\hbar^2 |\psi\rangle$

Since $|\psi\rangle = \alpha_1 |0\rangle|0\rangle + \alpha_2 |0\rangle|1\rangle + \alpha_3 |1\rangle|0\rangle + \alpha_4 |1\rangle|1\rangle$ and same for $\hat{S}_2^2$.

$\Rightarrow$ So, Can replace S_1^2 & S_2^2 w/ constants $\frac{3}{4}\hbar^2$

$\Rightarrow$ We see that $\hat{H} = D\,\hat{S}_T^2 - F$, D, F = constant > 0

$\Rightarrow$ What state $|\psi\rangle$ has smallest $\langle \psi | S_T^2 | \psi \rangle$??

$\Rightarrow$ Need $|\psi\rangle$ such that $\langle \psi | S_T^2 | \psi \rangle = 0$!

$\Rightarrow$ Hypothesis : $|\psi\rangle_0 = \frac{1}{\sqrt{2}}\left[|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2\right]$

is the g-state! i.e., $\langle\psi_0| S_T^2 |\psi_0\rangle = 0$,

the minimum value.

Prove : Must calculate $\langle\psi_0| S_T^2 |\psi_0\rangle =$

$$\frac{1}{\sqrt{2}}\left[\langle 0|\langle 1| - \langle 1|\langle 0|\right]\cdot\left[\hat{S}_1^2 + \hat{S}_2^2 + 2\,\vec{S}_2\cdot\vec{S}_1\right]\cdot\frac{1}{\sqrt{2}}\left[|0\rangle|1\rangle - |1\rangle|0\rangle\right]$$

$\Rightarrow$ Use $\vec{S}_2\cdot\vec{S}_1 = S_{2x}S_{1x} + S_{2y}S_{1y} + S_{2z}S_{1z}$

$S_{2x} \rightarrow \frac{1}{2}(S_{+2} + S_{-2})$

$S_{2y} \rightarrow \frac{1}{2i}(S_{+2} - S_{-2})$

H.W.

$\Rightarrow$ Can show $\langle S_T^2\rangle_0 = 0 \Rightarrow |\psi\rangle_0$ is zero total spin state, the g-state!

So, experimentally can create Bell state by putting 2 spins next to each other, and provide a perturbation so they fall into g-state!!

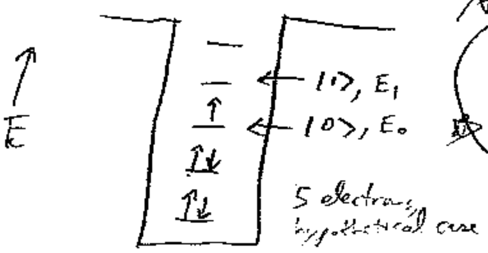
Now let's talk about a new qubit system!

<u>ATOMS!!</u>

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

<u>Quick answer</u>: 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!

[could think of it as a spin qubit, but let's consider electronic states.]



State of valence electron $= |\psi\rangle$
$\Rightarrow |\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

<u>Question</u>: How Measure and manipulate this qubit?
How do we control $|\psi\rangle$?

<u>Answer</u>: Apply a Hamiltonian!! Apply an external field that leads to some $\hat{H}$.
(Laser Light!!)
$\Rightarrow$ SOLVE SCHR. EQ'N !!

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle ! \qquad |\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$$

$\hat{H}$ allows us to change $|\psi\rangle \longrightarrow |\psi\rangle'$

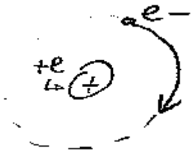
<u>NOTE</u>: If we keep our focus on only <u>one</u> electron hopping between 2 states then this problem is <u>identical</u> to the spin-½ problem! Have to relabel some quantities, but basic results the same!

<u>Qubit state</u> $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ can be thought of as a vector on Bloch sphere, even though it's not spin!!

$\Rightarrow$ To move forward we must have a better idea of what $|0\rangle$ & $|1\rangle$ actually are, and how do we compute $\hat{H}$ and its action on $|\psi\rangle$?

$|0\rangle$ & $|1\rangle \rightarrow$ Atomic Energy Levels for a single electron

$|0\rangle$ & $|1\rangle$ are the energy eigenstates for an electron orbiting a nucleus.



$$\left.\begin{aligned} \hat{H}_0 |0\rangle &= E_0 |0\rangle \\ \hat{H}_0 |1\rangle &= E_1 |1\rangle \end{aligned}\right\} \leftarrow \text{What's } H_0, E_0, E_1, |0\rangle |1\rangle ??$$

Where $\hat{H}_0$ is the Hamiltonian describing this.

$\Rightarrow$ What is $\hat{H}_0$ for simplest Atom, hydrogen?

$\hat{H}_0$ comes from classical energy: $E = KE + P.E.$

$$E = p^2/2m + \frac{-e^2}{r}$$

attractive potential

$$\Rightarrow \hat{H}_0 = \frac{\hat{P}^2}{2m} - \frac{e^2}{r}$$

$\Rightarrow$ Must solve Schr. eq'n: $H_0|\psi_n\rangle = E_n|\psi_n\rangle$

$$\left(\frac{\hat{P}^2}{2m} - \frac{e^2}{r}\right)\psi_n(\vec{r}) = E_n \psi_n(\vec{r})$$

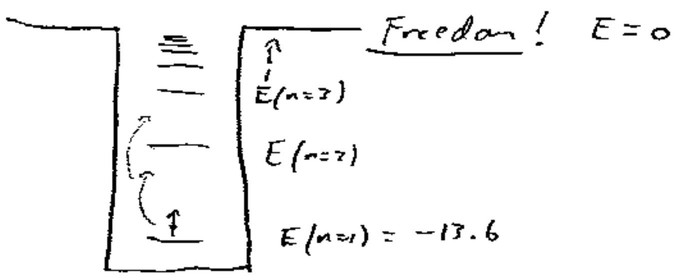
This is slightly tedious to solve, to see sol'n $\Rightarrow$ take a Q.M. course like 137A.

(if we ignore spin!) $\qquad E_{nlm} = \frac{-13.6eV}{n^2}$

$\boxed{\text{Answer}}$: $\psi_n(\vec{r}) = \psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_{lm}(\theta, \phi)$

Electron moves in 3 dimensions $\Rightarrow$ get 3 Quantum #'s: n, l, m

n = princ. Q. number, since it controls energy
l = magnitude of orbital ang. momentum, $\hat{L}^2$ (like "s" for spin & S^2)
m = z-component of $\vec{L}$ ⇒ $\hat{L}_z$ (like m for S_z w/ spin)



$$E_{n\ell m} = \frac{-13.6}{n^2}$$

The energy levels can be degenerate, and some degeneracies can be lifted by various perturbations.
LET'S IGNORE ALL THIS DETAIL, that is a topic for a straight Q.M. course (which this isn't!)

Even though the electron can bounce between an ∞ # of states, let's assume that it spends most of its time hopping between just 2 states and ignore the others. This is a surprisingly good approximation!

$$\Rightarrow \quad |0\rangle = R_{n\ell}(r)\,Y_{\ell m}(\theta,\phi) \text{ for some } n,\ell,m;\ E_0 = E_{n\ell m}$$
$$|1\rangle = R_{n'\ell'}(r)\,Y_{\ell' m'}(\theta,\phi) \text{ for some } n',\ell',m';\ E_1 = E_{n'\ell' m'}$$

[the details do matter for performing accurate calculations]

OK, now we know what $|0\rangle$ & $|1\rangle$ look like.
⇒ What does $\hat{H}$ look like in the 2-d subspace defined by $|0\rangle$ & $|1\rangle$??

This is a slightly awkward Question, since I already told you that for an "unperturbed" atom
$\Rightarrow \hat{H} = \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{-e^2}{r}$,

So, you might say "$\hat{H}$ is a function of position, $\vec{r}$"
Or, you might say "$\hat{H}$ is a 2×2 matrix"

Both of these answers are correct! How do we reconcile them?
<u>KEY PT</u>: $\hat{H}$ looks DIFFERENT for DIFFERENT basis!!

If we're talking about motion of electron through space around the nucleus, then a convenient basis is $\{|\vec{r}\rangle\}_{\vec{r}}$, the set of all points $\vec{r}$ throughout space.
Then $\hat{H} = f(\vec{r})$, a function of $\vec{r}$ $\Rightarrow$ could construct an ∞ 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 2 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:

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \qquad \underset{\#1}{|0\rangle}, \ \underset{\#2}{|1\rangle}$$

[<u>Moral of story</u>: Choose your basis wisely!!]

$\Rightarrow$ <u>Find Matrix elements</u>:

$$H_{11} = \langle 0 | \hat{H}_0 | 0 \rangle = E_0 \langle 0|0\rangle = E_0$$
$$H_{12} = \langle 0 | \hat{H}_0 | 1 \rangle = E_1 \langle 0|1\rangle = 0$$
$$H_{21} = \langle 1 | \hat{H}_0 | 0 \rangle = E_0 \langle 1|0\rangle = 0$$
$$H_{22} = \langle 1 | \hat{H}_0 | 1 \rangle = E_1 \langle 1|1\rangle = E_1$$

$$\Rightarrow \hat{H}_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}$$

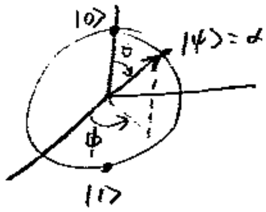
[this is equivalent to spin in B-field!! $\vec{B} = B_0\hat{z}$; ΔE ; $\hat{H} = -\vec{\mu}\cdot\vec{B} = \frac{e}{m}B_0\hat{S}_z$; $\hat{H} = \frac{e\hbar}{2m}\begin{pmatrix} B_0 & 0 \\ 0 & -B_0 \end{pmatrix}$]

$\Rightarrow$ This describes state of an electron in an unperturbed atom:

If $|\psi(t=0)\rangle = \alpha|0\rangle + \beta|1\rangle \Rightarrow |\psi(t)\rangle = e^{-i\hat{H}_0 t/\hbar}|\psi(0)\rangle$

$$\Rightarrow |\psi(t)\rangle = \alpha|0\rangle e^{-iE_0 t/\hbar} + \beta|1\rangle e^{-iE_1 t/\hbar}$$

Geometrically, this can be interpreted as a vector on Bloch sphere, just like for spin (even though it's NOT SPIN!)



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

Role of $\vec{B}$-field $(B_0\hat{z})$ is now played by energy difference $E_1 - E_0$

If $|\psi(0)\rangle$ starts off at (θ_0, ϕ_0) $\Rightarrow$ at time t later
$\Rightarrow |\psi(t)\rangle$ has rotated by $\Delta\phi$ around $\hat{z}$ axis at angular frequency $\omega_0 = \frac{E_1 - E_2}{\hbar}$ (like $\omega_0 = \frac{eB_0}{m}$)

<u>BUT</u>, we see that $\hat{H} = \hat{H}_0$ will never induce "spin-flips", i.e. change ratio between $|0\rangle$ & $|1\rangle$ (i.e., change θ!)
How do we do that??