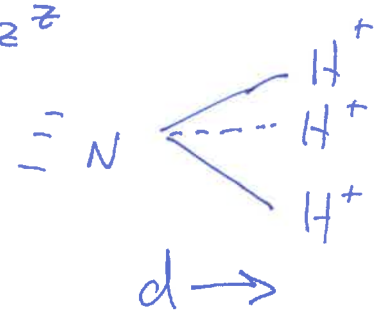
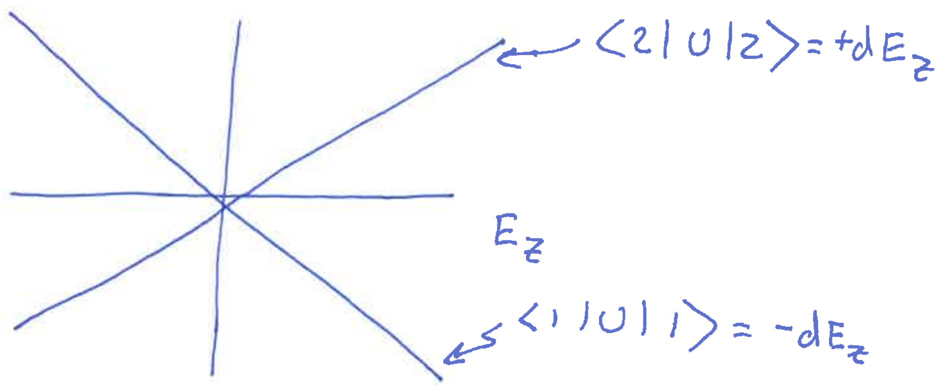
Two-Level Systems, Part III

We can make $[\Pi, H] \neq 0$ by applying an external field $\vec{E} = E_z \hat{z}$

$|L\rangle \approx |1\rangle$:



$U = -\vec{d} \cdot \vec{E}$



Call $\epsilon \equiv dE_z$ (Signed quantity)

$H = H_0 + U$

In $|1\rangle, |2\rangle$ basis $\quad H = \begin{pmatrix} E_0 - \epsilon & -\Delta \\ -\Delta & E_0 + \epsilon \end{pmatrix}$

2-State Math

- Find eigenvalues of this 2-level system.

$$H = E_0 \mathbb{1} + \underbrace{\begin{pmatrix} -\epsilon & -\Delta \\ -\Delta & +\epsilon \end{pmatrix}}_{h}$$

(This trick is useful when all elements of H are real)

$\boxed{0}$ - Now just diagonalize h

$$\begin{pmatrix} -\epsilon & -\Delta \\ -\Delta & \epsilon \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_h \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\begin{aligned} -\epsilon\alpha - \Delta\beta &= E_\ell\,\alpha \\ -\Delta\alpha + \epsilon\beta &= E_\ell\,\beta \end{aligned} \Rightarrow \begin{aligned} -\Delta\beta &= (E_\ell + \epsilon)\alpha \\ -\Delta\alpha &= (E_\ell - \epsilon)\beta \end{aligned}$$

$$\frac{\alpha}{\beta} = \frac{-\Delta}{E_\ell + \epsilon} = \frac{E_\ell - \epsilon}{-\Delta}$$

$$\Rightarrow (E_\ell + \epsilon)(E_\ell - \epsilon) = \Delta^2 \Rightarrow E_\ell = \pm \overbrace{\sqrt{\Delta^2 + \epsilon^2}}^{\equiv \text{ positive root}}$$

$$= E_\ell^2 - \epsilon^2$$

Eigenvalues of H:

$$E = E_0 + E_\ell = \boxed{E_0 \pm \sqrt{\Delta^2 + \epsilon^2}}$$

Call them E_g, E_u
"ground" "upper"

Eigenvectors of H found by plugging in those energies:

$$\frac{\alpha}{\beta} = \frac{-\Delta}{\epsilon \pm \sqrt{\Delta^2 + \epsilon^2}}$$

In $|1\rangle, |2\rangle$ basis

$$\boxed{|\varphi_g\rangle = N_g \begin{pmatrix} -\Delta \\ \epsilon - \sqrt{\Delta^2 + \epsilon^2} \end{pmatrix} \qquad |\varphi_u\rangle = N_u \begin{pmatrix} -\Delta \\ \epsilon + \sqrt{\Delta^2 + \epsilon^2} \end{pmatrix}}$$

i.e. $|\varphi_g\rangle = (N_g)\Big(-\Delta \underset{|L\rangle}{\underset{\Updownarrow}{|1\rangle}} + (\epsilon - \sqrt{\Delta^2+\epsilon^2}) \underset{|R\rangle}{\underset{\Updownarrow}{|2\rangle}}\Big)$

Alternate (one of a few) approach to diagonalization.

$$H|\psi\rangle = \lambda|\psi\rangle \Rightarrow (H-\lambda\mathbb{1})|\psi\rangle = 0 \Rightarrow \mathrm{Det}(H-\lambda\mathbb{1}) = 0$$

This is called "characteristic eqn"

Eigenvalues λ are given by determinant equation

$$\begin{vmatrix} E_0-\epsilon-\lambda & -\Delta \\ -\Delta & E_0+\epsilon-\lambda \end{vmatrix} = 0$$

$$\Rightarrow (E_0-\epsilon-\lambda)(E_0+\epsilon-\lambda) - \Delta^2 = 0$$

- Quadratic eqn for λ, which is easy.

- Equivalent to what we did before.

Check a few properties:

Orthogonality

(if Δ or $\epsilon \neq 0$)

H is non-degenerate, so $\langle \varphi_u | \varphi_g \rangle$ should be 0

$$\langle \varphi_u | \varphi_g \rangle = (N_u N_g)(\Delta^2 + \epsilon^2 - (\Delta^2 + \epsilon^2)) = 0 \quad \checkmark$$

Limit of strong $\vec{E}$ pointing right

$$\epsilon > 0, \quad |\epsilon| \gg \Delta, \quad \sqrt{\Delta^2+\epsilon^2} = \epsilon\sqrt{1+\frac{\Delta^2}{\epsilon^2}} \approx (\epsilon)\left(1+\frac{1}{2}\frac{\Delta^2}{\epsilon^2}\right) = \epsilon + \frac{\Delta^2}{2\epsilon}$$

$$|\varphi_g\rangle \to N_g \begin{pmatrix} -\Delta \\ -\frac{\Delta^2}{2\epsilon} \end{pmatrix} \to e^{i\phi} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle$$

uninteresting phase factor $\vec{d} \rightarrow$

$$|\varphi_u\rangle \to N_u \begin{pmatrix} -\Delta \\ 2\epsilon \end{pmatrix} \to \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |2\rangle$$

(Oriented molecule)

Limit of strong $\vec{E}$ pointing left

$$\epsilon < 0, \quad |\epsilon| \gg \Delta, \quad \sqrt{\Delta^2+\epsilon^2} = |\sqrt{\epsilon^2}|\sqrt{1+\frac{\Delta^2}{\epsilon^2}} \cong (-\epsilon)\left(1+\frac{1}{2}\frac{\Delta^2}{\epsilon^2}\right) = \underbrace{-\epsilon - \frac{\Delta^2}{2\epsilon}}_{>0 \; \checkmark}$$

$$|\varphi_g\rangle \to N_g \begin{pmatrix} -\Delta \\ 2\epsilon \end{pmatrix} \to \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |2\rangle$$

(Oriented too, but s.t. g.s. points opposite direction)

$$|\varphi_u\rangle \to N_u \begin{pmatrix} -\Delta \\ -\frac{\Delta^2}{2\epsilon} \end{pmatrix} \to \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |1\rangle$$

Limit of weak field

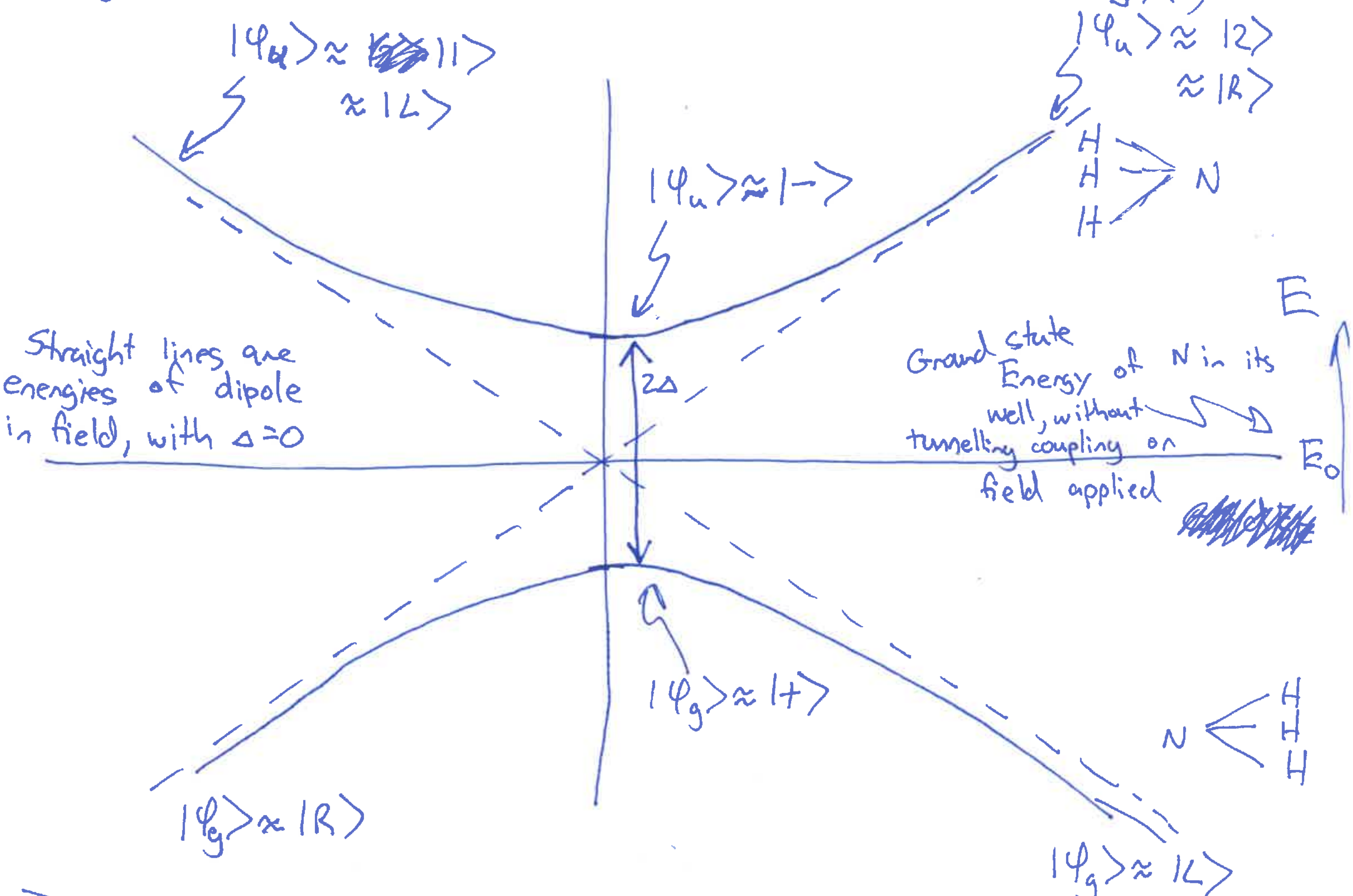
$$|\epsilon| \ll \Delta$$

$$|\varphi_g\rangle \longrightarrow N_g \begin{pmatrix} -\Delta \\ -\Delta \end{pmatrix} = |+\rangle$$

$$|\varphi_u\rangle \longrightarrow N_u \begin{pmatrix} -\Delta \\ \Delta \end{pmatrix} = |-\rangle$$

$E_u = E_0 + \sqrt{\Delta^2 + \epsilon^2}$
$E_g = E_0 - \sqrt{\Delta^2 + \epsilon^2}$

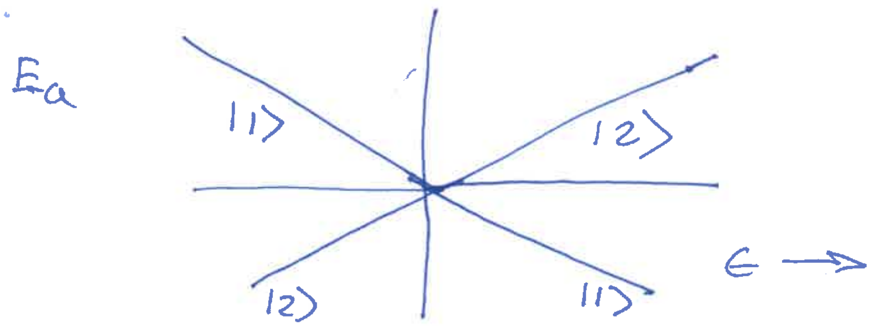
$E_u > E_g$ for all ϵ. (Lower eigenstate for all ϵ is $|\varphi_g\rangle$.)



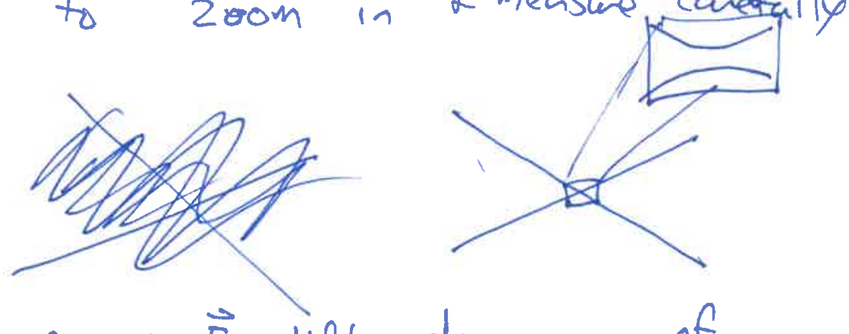
$\Rightarrow$ – Field orients the eigenstates if it is strong enough

- Notice how as we change the field strength, the character of the ~~upper~~ ground eigenstate changes smoothly from $|R\rangle \to |+\rangle \to |L\rangle$

- Without tunelling, we would have a crossing



- But with tunnelling interaction, we have an "avoided crossing". Common story in QM. ~~Sometimes~~ Usually there is some interaction. Sometimes have to zoom in + measure carefully to see it.



- Notice that either Δ or $\vec{E}$ lifts degeneracy of N getting to choose between sitting in two identical wells. With either term in H, degeneracy is broken + eigenstates of H are unique. $\langle \psi_s | \vec{d} | \psi_s \rangle \Rightarrow$

- Notice that at $|\vec{E}| = 0$, $\langle + | \vec{d} | + \rangle = 0$. No dipole moment until you induce it by turning on field. Prefer to say "molecule frame dipole moment" rather than "permanent dipole moment"

- However, if Π is not a real symmetry of nature, then $\langle \vec{d} \rangle \neq 0$ in eigenstates.

$\Rightarrow$ Search for EDM (fundamental electric dipole moment) of electrons, neutrons, molecules, etc.

would also be indications of time-reversal symmetry violation

Finding eigenvalues of the general 2-level system is very easy, as shown above. However, the eigenstate math, although straightforward, is ugly. So, for instance to see time dependence, it is often preferable to express the results in terms of mixing angles Θ & ϕ, where the results are more concise.

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(H_{11}+H_{22}) & 0 \\ 0 & \frac{1}{2}(H_{11}+H_{22}) \end{pmatrix} + \begin{pmatrix} \frac{1}{2}(H_{11}-H_{22}) & H_{12} \\ H_{21} & -\frac{1}{2}(H_{11}-H_{22}) \end{pmatrix}$$

$$= \frac{1}{2}(H_{11}+H_{22})\mathbb{1} + \frac{1}{2}(H_{11}-H_{22})K, \quad \text{where } K = \begin{pmatrix} 1 & \frac{2H_{12}}{H_{11}-H_{22}} \\ \frac{2H_{21}}{H_{11}-H_{22}} & -1 \end{pmatrix}$$

- Eigenvectors of K are also eigenvectors of H
- Eigenenergies are $E_\pm = \frac{1}{2}(H_{11}+H_{22}) + \frac{1}{2}(H_{11}-H_{22})K_\pm$ where $K_\pm$ are eigenvalues of K
- Define

$$\tan\Theta = \frac{2|H_{21}|}{H_{11}-H_{22}}, \quad 0 \le \Theta < \pi$$

$$H_{21} = |H_{21}|e^{i\phi}, \quad 0 \le \phi < 2\pi$$

$$\Rightarrow \quad K = \begin{pmatrix} 1 & \tan\theta\, e^{-i\phi} \\ \tan\theta\, e^{i\phi} & -1 \end{pmatrix}$$

Eigenvalues of K are given by

$$\mathrm{Det}\left[K - K\,\mathbb{1}\right] = 0$$

$$\Rightarrow \quad (1-K)(-1-K) - \tan^2\theta = 0$$

$$-1 + K^2 - \tan^2\theta = 0$$

$$K^2 = 1 + \tan^2\theta = \frac{1}{\cos^2\theta}$$

$$\Rightarrow \quad \boxed{K_\pm = \pm\frac{1}{\cos\theta}}$$

$$K^2 = \frac{4|H_{21}|^2}{(H_{11}-H_{22})^2} + 1$$

$$\Rightarrow \quad \boxed{K_\pm = \frac{\pm\sqrt{(H_{11}-H_{22})^2 + 4|H_{21}|^2}}{H_{11}-H_{22}}}$$

$$\boxed{E_\pm = \frac{1}{2}(H_{11}+H_{22}) \pm \frac{1}{2}\sqrt{(H_{11}-H_{22})^2 + 4|H_{12}|^2}}$$

Eigenvectors:

For K_+,

$$\begin{pmatrix} 1 & \tan\theta\, e^{-i\phi} \\ \tan\theta\, e^{i\phi} & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\cos\theta} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\Rightarrow \left(1 - \frac{1}{\cos\theta}\right) a + \tan\theta\, e^{-i\phi}\, b = 0$$

(apologies for trig identities...)

$$\Rightarrow -\left(\sin\frac{\theta}{2}\, e^{i\frac{\phi}{2}}\right) a + \left(\cos\frac{\theta}{2}\, e^{-i\frac{\phi}{2}}\right) b = 0$$

$$\Rightarrow \boxed{|\varphi_+\rangle = \cos\frac{\theta}{2}\, e^{-i\phi/2}|\varphi_1\rangle + \sin\frac{\theta}{2}\, e^{i\phi/2}|\varphi_2\rangle}$$

(normalized)

And similarly we get

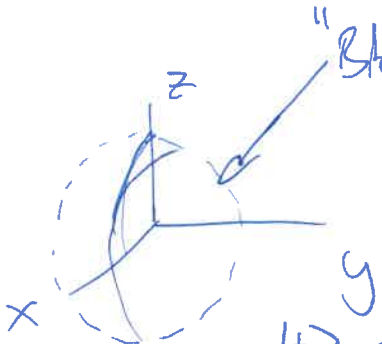
$$\boxed{|\varphi_-\rangle = -\sin\frac{\theta}{2}\, e^{-i\phi/2}|\varphi_1\rangle + \cos\frac{\theta}{2}\, e^{i\phi/2}|\varphi_2\rangle}$$

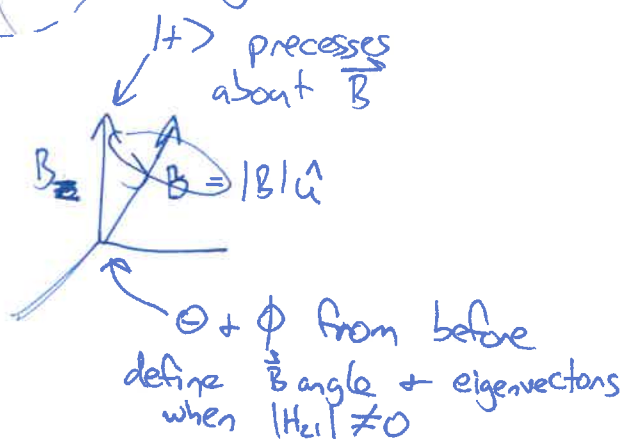
So often we will parameterize ~~coup~~ off-diagonal coupling in terms of mixing angles, e.g. neutrinos.

Fictitious B-Fields

- Representation in terms of angles suggests the 2-level problem might map onto same problem with same real-space angles.

- Yes. 2-level systems dynamics are completely equivalent to a spin-$\frac{1}{2}$ in a B field.





$$|\varphi_1\rangle \leftrightarrow |+\rangle$$
$$|\varphi_2\rangle \leftrightarrow |-\rangle$$
$$|\varphi_+\rangle \leftrightarrow |+\rangle_u$$
$$|\varphi_-\rangle \leftrightarrow |-\rangle_u$$
$$E_+ - E_- \leftrightarrow \hbar\omega$$
$$H_{11} - H_{22} \leftrightarrow -\gamma\hbar B_z$$
$$|H_{21}| \leftrightarrow -\gamma\hbar B_\perp / 2$$

Even resonant + off-resonant drives map.

e.g., when $B_\perp = 0$

$|+\rangle \to |+\rangle_x$ by "$\pi/2$" pulse. Works in NMR.

equivalent can be done

$$|\varphi_1\rangle \to \frac{1}{\sqrt{2}}\left(|\varphi_1\rangle + |\varphi_2\rangle\right)$$