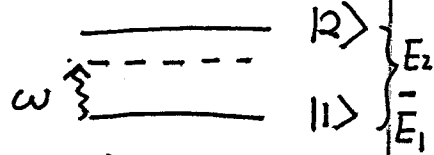


Lect 21 Time-dependent problem — 2 energy levels

§ Two energy level coupled to AC field

$$H = H_0 + V(t)$$



$$H_0 = E_1 |1\rangle\langle 1| + E_2 |2\rangle\langle 2|, \text{ and } V(t) = \gamma e^{i\omega t} |1\rangle\langle 2| + \gamma e^{-i\omega t} |2\rangle\langle 1|$$

$|1\rangle$, and $|2\rangle$ are energy levels, $V(t)$ can be considered as a driven laser with a frequency ω : $\gamma = \langle 1| e^{i\vec{r}\cdot\vec{E}} |2\rangle$. If the coupling matrix element is large, or $E_2 - E_1 \approx \omega$, we cannot use the linear order perturbation theory in last lecture. For the case of 2-energy levels we can solve it exactly.

$$|\psi(t)\rangle = C_1(t) e^{-iE_1 t/\hbar} |1\rangle + C_2(t) e^{-iE_2 t/\hbar} |2\rangle$$

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} C_1(t) e^{-iE_1 t/\hbar} |1\rangle + i\hbar \frac{\partial}{\partial t} C_2(t) e^{-iE_2 t/\hbar} |2\rangle + E_1 C_1(t) e^{-iE_1 t/\hbar} |1\rangle + E_2 C_2(t) e^{-iE_2 t/\hbar} |2\rangle$$

$$(H_0 + V(t)) |\psi(t)\rangle = C_1(t) E_1 e^{-iE_1 t/\hbar} |1\rangle + C_2(t) E_2 e^{-iE_2 t/\hbar} |2\rangle + C_1(t) V(t) e^{-iE_1 t/\hbar} |1\rangle + C_2(t) V(t) e^{-iE_2 t/\hbar} |2\rangle$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} C_1(t) e^{-iE_1 t/\hbar} |1\rangle + i\hbar \frac{\partial}{\partial t} C_2(t) e^{-iE_2 t/\hbar} |2\rangle$$

$$= C_1(t) V(t) e^{-iE_1 t/\hbar} |1\rangle + C_2(t) V(t) e^{-iE_2 t/\hbar} |2\rangle$$

$$= C_1(t) \gamma e^{-i\omega t - iE_1 t/\hbar} |2\rangle + C_2(t) \gamma e^{i\omega t - iE_2 t/\hbar} |1\rangle$$

$$\begin{cases} i\hbar \frac{\partial}{\partial t} C_1(t) = \gamma e^{i(\omega - \frac{E_2 - E_1}{\hbar})t} C_2(t) = \gamma e^{-i\Delta\omega t} C_2(t) \\ i\hbar \frac{\partial}{\partial t} C_2(t) = \gamma e^{-i(\omega - \frac{E_2 - E_1}{\hbar})t} C_1(t) = \gamma e^{i\Delta\omega t} C_1(t) \end{cases}$$

$$\Delta\omega = \frac{E_2 - E_1 - \omega}{\hbar}$$

$$\begin{aligned} \frac{d^2}{dt^2} C_1(t) &= \frac{\gamma}{i\hbar} [-i\Delta\omega] e^{-i\Delta\omega t} C_2(t) + \frac{\gamma}{i\hbar} e^{-i\Delta\omega t} \frac{d}{dt} C_2(t) \\ &= -\frac{\Delta\omega}{\hbar} i\hbar \frac{d}{dt} C_1(t) + \frac{\gamma}{i\hbar} e^{-i\Delta\omega t} \frac{1}{i\hbar} \gamma e^{i\Delta\omega t} C_1(t) \end{aligned}$$

$$\Rightarrow \boxed{\frac{d^2}{dt^2} C_1(t) + i\Delta\omega \frac{d}{dt} C_1(t) + \frac{\gamma^2}{\hbar^2} C_1(t) = 0}$$

The characteristic Eq $\lambda^2 + i\Delta\omega\lambda + \frac{\gamma^2}{\hbar^2} = 0 \Rightarrow \lambda_{1,2} = \frac{-i\Delta\omega}{2} \pm i\sqrt{\left(\frac{\Delta\omega}{2}\right)^2 + \left(\frac{\gamma}{\hbar}\right)^2}$

define $\Omega = \left[\left(\frac{\gamma}{\hbar}\right)^2 + \left(\frac{\Delta\omega}{2}\right)^2 \right]^{1/2}$

$$\begin{aligned} \Rightarrow C_1(t) &= \left[A e^{i\Omega t} + B e^{-i\Omega t} \right] e^{-i\frac{\Delta\omega}{2}t} \quad A, B \text{ to be determined} \\ C_2(t) &= \frac{\hbar}{\gamma} \left[-(\Omega - \frac{\Delta\omega}{2}) A e^{i\Omega t} + (\Omega + \frac{\Delta\omega}{2}) B e^{-i\Omega t} \right] e^{i\frac{\Delta\omega}{2}t} \end{aligned}$$

Consider the initial condition $C_1(0)=1$, and $C_2(0)=0$

we set $\begin{cases} A + B = 1 \\ -(\Omega - \frac{\Delta\omega}{2})A + (\Omega + \frac{\Delta\omega}{2})B = 0 \end{cases} \Rightarrow \begin{cases} A = \frac{1}{2} + \frac{\Delta\omega}{4\Omega} \\ B = \frac{1}{2} - \frac{\Delta\omega}{4\Omega} \end{cases}$

$$\Rightarrow C_1(t) = \frac{-i\hbar}{\gamma\Omega} \left[\Omega^2 - \left(\frac{\Delta\omega}{2}\right)^2 \right] \sin\Omega t e^{-i\frac{\Delta\omega}{2}t} = \frac{-i\gamma/\hbar}{\Omega} \sin\Omega t e^{i\frac{\Delta\omega}{2}t}$$

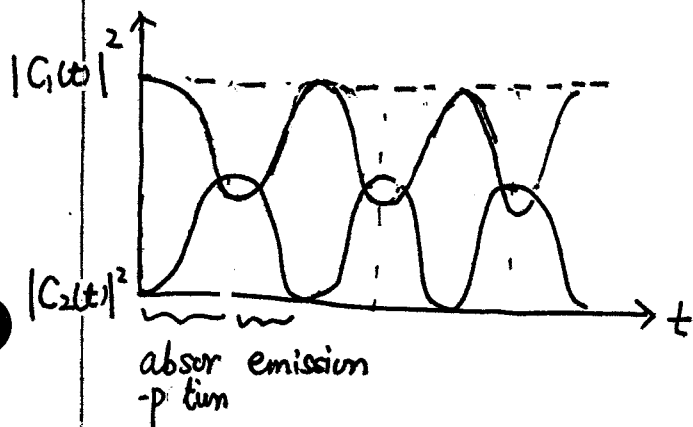
$$|C_2(t)|^2 = \frac{(\gamma/\hbar)^2}{(\gamma/\hbar)^2 + (\frac{\Delta\omega}{2})^2} \sin^2 \Omega t = \frac{(\gamma/\hbar)^2}{\Omega^2} \sin^2 \Omega t$$

$$C_1(t) = \left[\cos \Omega t + \frac{i \Delta\omega}{2\Omega} \sin \Omega t \right] e^{-i \frac{\Delta\omega}{2} t}$$

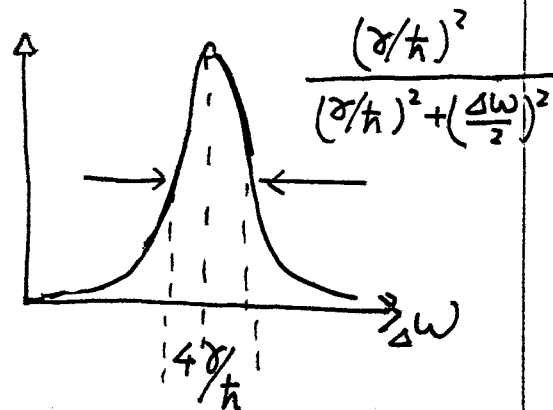
$$|C_1(t)|^2 = \cos^2 \Omega t + \left(\frac{\Delta\omega}{2\Omega} \right)^2 \sin^2 \Omega t = 1 - \frac{\Omega^2 - (\frac{\Delta\omega}{2})^2}{\Omega^2} \sin^2 \Omega t$$

$$= 1 - |C_2(t)|^2$$

IMPACT



the magnitude of $C_2(t)$



$\Delta\omega = 0$ is resonance point!

§ Bloch sphere picture for 2 energy level system:

Now the wavefunction $\psi(t) = \begin{pmatrix} C_1(t) e^{-iE_1 t/\hbar} \\ C_2(t) e^{-iE_2 t/\hbar} \end{pmatrix}$

define

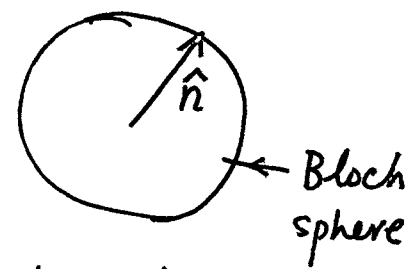
$$n_3 = |\psi_1|^2 - |\psi_2|^2$$

$$n_1 = \psi_1^* \psi_2 + \psi_2^* \psi_1$$

$$n_2 = -i \psi_1^* \psi_2 + i \psi_2^* \psi_1$$

$$\text{or } \vec{n} = \psi_\alpha^* \vec{\sigma}_{\alpha\beta} \psi_\beta$$

Ex check that $n_1^2 + n_2^2 + n_3^2 = 1$.



FORWARD

$$\begin{cases}
 n_3 = |C_1(t)|^2 - |C_2(t)|^2 \\
 n_1 = 2 \left[\text{Re} [C_1^*(t) C_2(t)] \cos \frac{(E_2 - E_1)t}{\hbar} + \text{Im} C_1^*(t) C_2(t) \sin \frac{(E_2 - E_1)t}{\hbar} \right] \\
 n_2 = -2 \text{Re} [C_1^*(t) C_2(t)] \sin \frac{E_2 - E_1}{\hbar} t + 2 \text{Im} C_1^*(t) C_2(t) \cos \frac{(E_2 - E_1)t}{\hbar}
 \end{cases}$$

The n_1, n_2 components have a fast rotation due to the frequency $E_2 - E_1$, which is the Lamer frequency. Now we change to the corotating frame with the Lamer frequency, and only focus on the

variation from $C_1(t)$ and $C_2(t)$.

This is called - rotating wave frame. In this frame,

$$\psi'(t) = \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} \rightarrow \begin{cases} n'_3 = n_3(t) \\ n'_1 = 2 \text{Re} C_1^*(t) C_2(t) \\ n'_2 = 2 \text{Im} C_1^*(t) C_2(t) \end{cases}$$

Spin magnetic Resonance / NMR

$$\vec{B} = B_0 \hat{z} + B_1 (\hat{x} \cos \omega t + \hat{y} \sin \omega t)$$

$$\vec{\mu} = \frac{e}{m_e c} \vec{S}$$

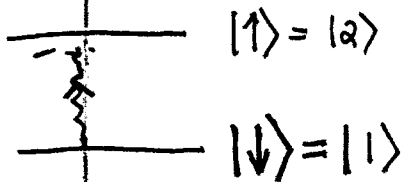
$$H = -\vec{\mu} \cdot \vec{B} = H_0 + V(t)$$

$$H_0 = \hbar \omega_{21} (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|) \quad \text{where } \omega_{21} = \frac{|e|B_0}{m_e c}$$

$$V(t) = \gamma \cos \omega t (|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) + \gamma \sin \omega t (-i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|)$$

$$= \gamma e^{-i\omega t} |\uparrow\rangle\langle\downarrow| + \gamma e^{i\omega t} |\downarrow\rangle\langle\uparrow|, \quad \text{where } \gamma = \frac{-e\hbar B_1}{2m_e c}, \quad e < 0.$$

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Then the problem is mapped back to previous

one. ① If $B_1 = 0$, i.e. $\gamma = 0$, then $|C_{\uparrow}(t)|^2 = \text{const}$,

spin only do precessions. $|C_{\downarrow}(t)|^2 = \text{const}$

② If $B_1 \neq 0$, i.e. $\gamma \neq 0$, $|C_{\uparrow}(t)|^2$ and $|C_{\downarrow}(t)|^2$ varies according to

$$\Omega = \left[\left(\frac{\gamma}{\hbar} \right)^2 + \left(\frac{\Delta\omega}{2} \right)^2 \right]^{1/2}$$

There're spin flip process!

• If for a linearly oscillating magnetic field, we can decompose it into a counter clockwise / clockwise part

$$2B_1 \hat{x} \cos \omega t = B_1 (\hat{x} \cos \omega t + \hat{y} \sin \omega t) + B_1 (\hat{x} \cos \omega t - \hat{y} \sin \omega t)$$

$$= \gamma (e^{-i\omega t} |\uparrow\rangle\langle\downarrow| + e^{i\omega t} |\downarrow\rangle\langle\uparrow|) + \gamma (e^{i\omega t} |\uparrow\rangle\langle\downarrow| + e^{-i\omega t} |\downarrow\rangle\langle\uparrow|)$$

$$i\hbar \frac{\partial}{\partial t} C_{\downarrow}(t) e^{-iE_1 t/\hbar} |\downarrow\rangle + i\hbar \frac{\partial}{\partial t} C_{\uparrow}(t) e^{-iE_2 t/\hbar} |\uparrow\rangle$$

$$= C_{\downarrow}(t) V(t) e^{-iE_1 t/\hbar} |\downarrow\rangle + C_{\uparrow}(t) V(t) e^{-iE_2 t/\hbar} |\uparrow\rangle$$

$$V(t) = \gamma (e^{-i\omega t} |\uparrow\rangle\langle\downarrow| + e^{i\omega t} |\downarrow\rangle\langle\uparrow|) + \gamma (e^{i\omega t} |\uparrow\rangle\langle\downarrow| + e^{-i\omega t} |\downarrow\rangle\langle\uparrow|)$$

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$$\Rightarrow i\hbar \frac{\partial}{\partial t} C_{\downarrow}(t) e^{-iE_1 t/\hbar} |\downarrow\rangle + i\hbar \frac{\partial}{\partial t} C_{\uparrow}(t) e^{-iE_2 t/\hbar} |\uparrow\rangle$$

$$= C_{\downarrow}(t) [\gamma (e^{-i\omega t - iE_1 t/\hbar} + e^{i\omega t + iE_2 t/\hbar}) |\uparrow\rangle]$$

$$+ C_{\uparrow}(t) [\gamma (e^{i\omega t - iE_2 t/\hbar} + e^{-i\omega t - iE_1 t/\hbar}) |\downarrow\rangle]$$

$$\Rightarrow \begin{cases} i\hbar \frac{\partial}{\partial t} C_{\downarrow}(t) = \gamma [e^{i(\omega - \omega_{21})t} + e^{-i(\omega + \omega_{21})t}] C_{\uparrow}(t) \\ i\hbar \frac{\partial}{\partial t} C_{\uparrow}(t) = \gamma [e^{-i(\omega - \omega_{21})t} + e^{i(\omega + \omega_{21})t}] C_{\downarrow}(t) \end{cases}$$

In the case of $\omega \rightarrow \omega_{21}$, we can neglect the parts of $e^{\pm i(\omega + \omega_{21})t}$ which are fast oscillations, which can be dropped. In other words, B_0 already selects the handedness.