OPTI 570 LECTURE TU DEC 2

Last time: Atomic structure

$$H = H_0 + W_{FS} + W_{HF}$$

Zeeman effect

hydrogen $\underline{n=1}$

$$H = H_0 + W_{FS} + W_{HF} + W_{ZN}$$

$$W_{Zm} = -\vec{\mu}\cdot\vec{B}$$

$$\vec{\mu} = \frac{\mu_B}{\hbar}\left(-\underset{=0}{g_L}\vec{L} - \underline{g_S\vec{S}} + g_I \underbrace{\frac{m_e}{m_p}}_{\text{tiny, neglect}}\vec{I}\right)$$

μ_B - Bohr magneton

$\underline{n=1}$ $\quad L=0$

$$\vec{\mu} \approx \frac{2\mu_B\vec{S}}{\hbar}$$

$$\vec{B} = B_0\hat{z}$$

$$\underline{W_{ZN}} = -\frac{2\mu_B}{\hbar}B_0\cdot S_z = \underline{2\omega_0 S_z}, \quad \omega_0 = -\frac{\mu_B B_0}{\hbar}$$

$L=0 \Rightarrow J=S \Rightarrow W_{ZN} = 2\omega_0 J_z$

TP basis: $\{\,|\underset{m_S\,m_I}{++}\rangle, |+-\rangle, |-+\rangle, |--\rangle\,\}$

$$W_{ZN} \to 2\hbar\omega_0\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{pmatrix}$$

TAM basis $\{|F,m_F\rangle\}$, $\quad \{\,|1,1\rangle, |1,0\rangle, |0,0\rangle, |1,-1\rangle\,\}$

$$W_{ZN} \to \hbar\omega_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$W_{HF} + W_{ZN} \rightarrow \begin{pmatrix} \tilde{\epsilon} + \hbar\omega_0 & 0 & 0 & 0 \\ 0 & \tilde{\epsilon} & \hbar\omega_0 & 0 \\ 0 & \hbar\omega_0 & -3\tilde{\epsilon} & 0 \\ 0 & 0 & 0 & \tilde{\epsilon} - \hbar\omega_0 \end{pmatrix}$$

<u>eigenvalues</u>

$\tilde{\epsilon} + \hbar\omega_0$

$\tilde{\epsilon} - \hbar\omega_0$

$-\tilde{\epsilon} + \sqrt{4\tilde{\epsilon} + \hbar^2\omega_0^2}$

$-\tilde{\epsilon} - \sqrt{4\tilde{\epsilon} + \hbar^2\omega_0^2}$

<u>eigenstates</u>

$|F=1, m_F=1\rangle$

$|F=1, m_F=-1\rangle$

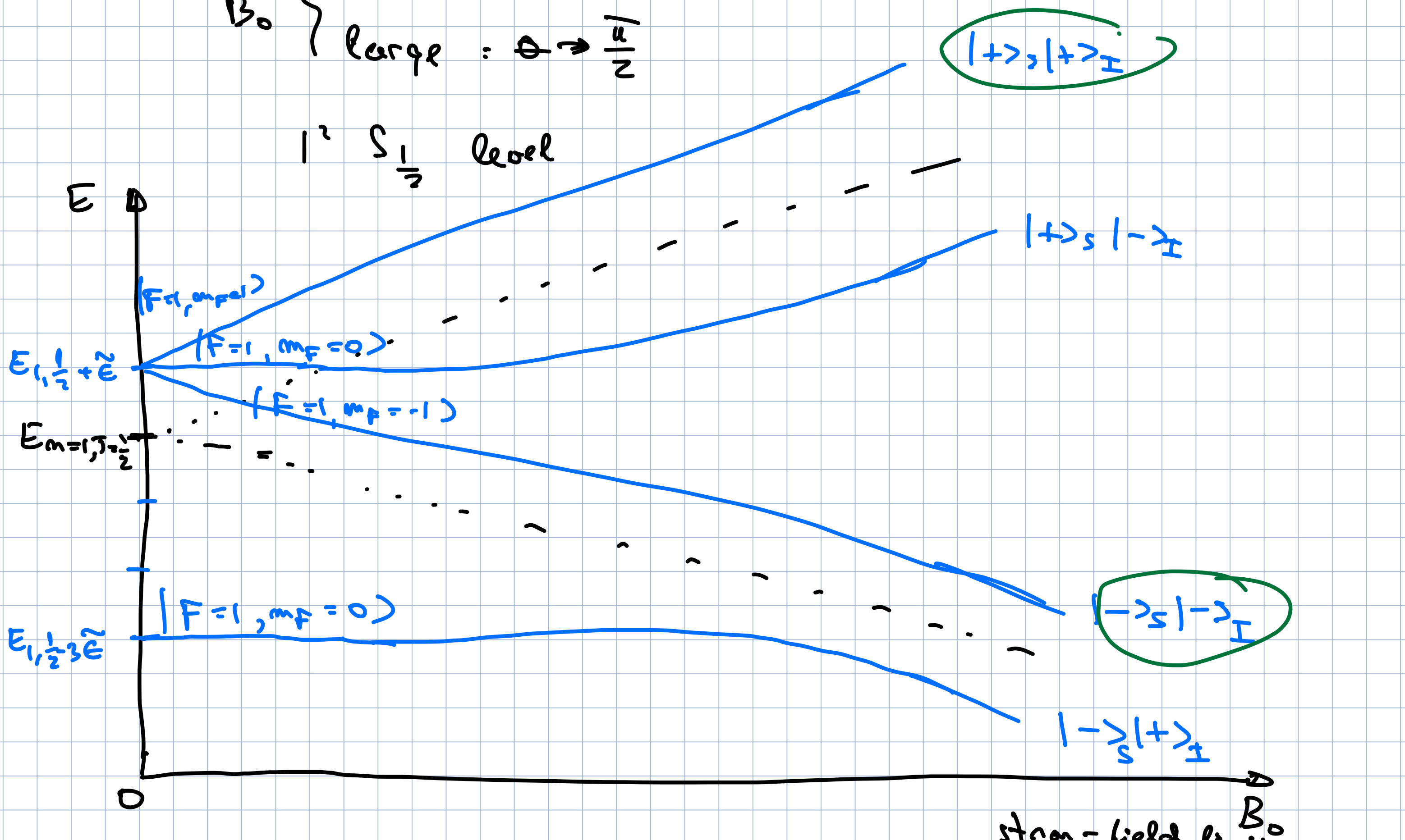
$\cos\frac{\theta}{2}|10\rangle + \sin\frac{\theta}{2}|00\rangle$

$\cos\frac{\theta}{2}|00\rangle - \sin\frac{\theta}{2}|10\rangle$

$$\theta = \mathrm{atan}\left(\frac{\hbar\omega_0}{2\tilde{\epsilon}}\right)$$

$$B_0 \begin{cases} \text{small} : \theta \rightarrow 0 \\ \text{large} : \theta \rightarrow \frac{\pi}{2} \end{cases}$$

$1^2 S_{\frac{1}{2}}$ level



strong-field limit

(Paschen-Back effect)

Time-Dependent Perturbation Theory (TDPT)

Known: • $H(t) = \underset{\sim}{H_0} + \lambda \hat{W}(t)$

• $|\psi(t)\rangle = \sum_m c_m(t=0)|\varphi_m\rangle$

Find: Probability of system being in some final state $|\varphi_f\rangle$ at some time t

$$P_f = |\langle \varphi_f | \psi(t)\rangle|^2$$

But... what do I do if I cannot calculate $|\psi(t)\rangle$?

USE TDPT

Method: $|\psi(t)\rangle = \sum_m c_m(t)|\varphi_m\rangle$

$$|\psi_E(t)\rangle = \sum_m \underbrace{c_m(t)\, e^{+iH_0 t/\hbar}} |\varphi_m\rangle$$

$$= \sum_m b_m(t)|\varphi_m\rangle$$

$$P_f(t) = |c_m(t)|^2 = |b_m(t)|^2$$

order of expansion

$$b_m(t) = b_m^{\boxed{(0)}}\underline{(t)} + \lambda b_m^{\boxed{(1)}}\underline{(t)} + \lambda^2 b_m^{(2)}\underline{(t)} + \ldots = \sum_{r=0}^{\infty} \lambda^r b_m^{(r)}(t)$$

$$i\hbar \frac{d}{dt}|\psi_E(t)\rangle = H_E(t)|\psi_E(t)\rangle$$

$$\uparrow \quad = \lambda U_0^{\dagger}(t)\,\hat{W}(t)\,U_0(t)$$

$$|\psi_E(t)\rangle = \sum_m \left(\sum_{r=0}^{\infty} \lambda^r b_m^{(r)}(t)\right) \underline{|\varphi_m\rangle}$$

Results:

0th order: $b_m^{(0)}(t) = b_m(t)$

ex: $|\psi(0)\rangle = \frac{1}{\sqrt{2}}|\varphi_0\rangle + \frac{1}{\sqrt{2}}|\varphi_2\rangle$

$$b_0^{(0)}(t) = b_0(0) = \frac{1}{\sqrt{2}}$$

$$b_2^{(0)}(t) = b_2(0) = \frac{1}{\sqrt{2}}$$

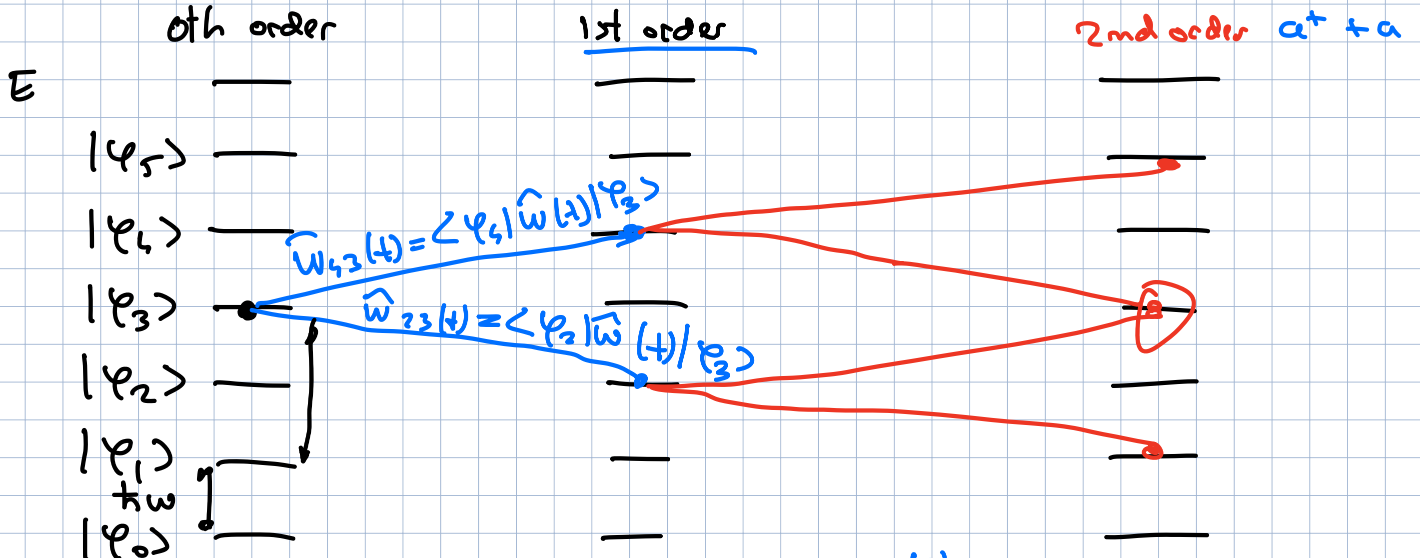
$$b_1^{(0)}(t) = 0$$

1st order :

$$\boxed{\lambda b_m^{(1)}(t) = \frac{1}{i\hbar} \sum_k \int_{t=0}^{t} dt\, e^{-i\omega_{mk}t'} \underbrace{\lambda \hat{W}_{mk}(t')}_{\lambda \hat{W}_{mk}(t') = \langle \varphi_m | \lambda \hat{W}(t') | \varphi_k \rangle} \underset{b_k(t_0)}{\underline{b_k^{(0)}(t)}}}$$

$$\omega_{mk} = \frac{E_m - E_k}{\hbar}$$

ex: 1D QHO , initial state $|\Psi(0)\rangle = \underline{|\varphi_3\rangle}$, $W \sim \underset{\sim}{x} \sin\left(\frac{\alpha t}{2}\right)$



ex: $|\Psi(0)\rangle = \overset{b_1^{(0)}(t)}{\sqrt{\frac{1}{5}}} |\varphi_1\rangle + \overset{b_2^{(0)}(t)}{\sqrt{\frac{4}{5}}} |\varphi_2\rangle$, $\lambda \hat{W}(t)$ perturbation

Determine prob. of the system to be found in state $|\varphi_3\rangle$ at time t to 1st order

need : $b_3(t) = \underbrace{b_3^{(0)}(t)}_{0} + \underbrace{\lambda b_3^{(1)}(t)}$

$$\lambda b_3^{(1)}(t) = \frac{\lambda}{i\hbar} \sum_{k=1}^{2} \int_{t'=0}^{t} dt'\, e^{i\omega_{3k}(t')} \hat{W}_{3k}(t') \left(\sqrt{\frac{1}{5}} \delta_{k1} + \sqrt{\frac{4}{5}} \delta_{k2} \right)$$

$$= \frac{\lambda}{i\hbar} \int_{t'=0}^{t} dt' \left(e^{i\omega_{31}t'} \underline{\hat{W}_{31}(t')} \sqrt{\frac{1}{5}} + e^{i\omega_{32}t'} \hat{W}_{32}(t') \sqrt{\frac{4}{5}} \right)$$

$$P_3^{(1)}(t) = |\lambda b_3^{(1)}(t)|^2$$

Let
- $\mathcal{H}_0$ is 1D QHO
- $W(t) = \lambda \hbar\omega \frac{x}{\sigma} \sin(\Omega t)$

$\omega_{31} = 2\omega \qquad \omega_{32} = \omega \qquad x = \frac{1}{\sqrt{2}}(a^{+} + a)$

$\lambda \hat{W} = W$

$\hat{W}_{31}(t) = 0$

$\underline{\hat{W}_{32}}(t) = \hbar\omega \left(\frac{1}{\sqrt{2}} < \underline{\varphi_3} | \underline{a^{+}} + a | \underline{\varphi_2} > \right) \sin(\Omega t)$

$= \hbar\omega \sqrt{\frac{3}{2}} \sin(\Omega t)$

$\lambda b_3^{(1)}(t) = \frac{\lambda}{i\hbar} \int_0^t dt' e^{i\omega t'} \cdot \hbar\omega \sqrt{\frac{3}{2}} \sin(\Omega t') \sqrt{\frac{4}{5}} =$

$\boxed{= -i\lambda\omega \sqrt{\frac{6}{5}} \int_0^t dt' e^{i\omega t'} \sin(\Omega t')}$

$\boxed{P_3^{(1)}(t) = \lambda^2 \omega^2 \frac{6}{5} \left| \int_0^t dt' e^{i\omega t'} \sin(\Omega t') \right|^2}$

$\underline{Q:}$ what about $P_4^{(1)}(t) = \underline{0}$.

to leading order what is $P_4(t)$?

$P_4^{(2)}(t) = ?$

<u>In general</u>:

$\lambda^r b_m^{(r)}(t) = \frac{1}{i\hbar} \sum_{k'} \int_{t_0}^{t} dt' e^{i\omega_{mk'} t'} [\lambda \hat{\omega}_{mk'}(t')][\lambda^{r-1} b_{k'}^{(r-1)}(t')]$

$P_4^{(2)}(t) = | \underbrace{b_4^{(0)}(0)}_{0} + \underbrace{\lambda b_4^{(1)}(t)}_{0} + \underline{\lambda^2 b_4^{(2)}(t)} |^2$

$\lambda^2 b_4^{(2)}(t) = \frac{1}{i\hbar} \int_0^t dt' e^{i\omega t'} \underbrace{< \varphi_4 | \lambda \hat{W}(t') | \varphi_3 >}_{\hbar\omega\sqrt{2}\sin(\Omega t'')} \boxed{\lambda b_3^{(1)}(t'')}$

$= -i\lambda^2 \omega\sqrt{2} \int_0^t dt' e^{i\omega t'} \sin(\Omega t') \cdot \boxed{\left(-i\omega \sqrt{\frac{6}{5}}\right) \cdot \int_0^{t'} dt'' e^{i\omega t''} \sin(\Omega t'')}$

$= -\lambda^2 \omega^2 \sqrt{\frac{12}{5}} \int_0^t \int_0^{t'} dt' dt'' e^{i\omega t'} e^{i\omega t''} \sin(\Omega t'') \sin(\Omega t')$

$$\boxed{P_4^{(2)}(t) = |\lambda^2 b_4^{(2)}(t)|^2}$$