Time-Indep PT

☒ Disc 6,7
☒ Hwk 6,7

Setup & derivation tech

- $\hat{\mathcal{H}} = \overset{\text{solvable}}{\mathcal{H}_0} + \varepsilon \overset{\text{small}}{\mathcal{H}'}$ $\longrightarrow$ $\{E_n^{(0)}, |n^{(0)}\rangle\}$ known & provide basis

EXPANSIONS

- $E_n = E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)} + \cdots$
- $|n\rangle = |n^{(0)}\rangle + \varepsilon |n^{(1)}\rangle + \varepsilon^2 |n^{(2)}\rangle + \cdots$

TECHNIQUES

★ Dial ε of Explicit Smallness

★ Equate powers of ε

★ Project onto e-states: $\langle m^{(0)}|n^{(j)}\rangle$ (of unpert. basis)

★ Hermiticity of $\mathcal{H}, \mathcal{H}_0, \mathcal{H}'$

$$\langle f|\mathcal{H}g\rangle = \langle \mathcal{H}f|g\rangle$$

SAME

Results 1:

non-degen states: w unique $E_n^{(0)}$

$E_n^{(1)}, |n^{(1)}\rangle, E_n^{(2)}$ → FORMULA SHEET

Results 2: degen states: $\{E_{\alpha_i}^{(0)}\} = E_D^{(0)}$ SAME VALUE

require $\langle \alpha_i^{(0)}|\mathcal{H}'|\alpha_j^{(0)}\rangle = 0$ when $i \neq j$

ie. that sub-matrix of $\mathcal{H}' \ni \{\text{degen } |\alpha_i\rangle\}$ is DIAG-ONAL

∴ switch basis $\{|\alpha_i^{(0)}\rangle\} \longrightarrow \{|\beta_i^{(0)}\rangle\}$

within degen subspace, if necessary

$$\mathcal{H}_0 = \left(\begin{array}{c|cc} E_1^{(0)} & & \\ \hline & \underline{E_\alpha^{(0)}} & \\ & & \underline{E_\alpha^{(0)}} \end{array}\right)$$

& $\mathcal{H}'$ in orig basis $= \left(\begin{array}{c|cc} \Gamma & \cdot & \cdot \\ \hline \cdot & a & b \\ \cdot & b^* & c \end{array}\right)$

NEW BASIS: $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $\underbrace{\left\{ |\beta\rangle = \begin{pmatrix} 0 \\ \bullet \\ \bullet \end{pmatrix}, \begin{pmatrix} 0 \\ \bullet \\ \bullet \end{pmatrix} \right\}}_{\text{STILL HAVE same unperturbed energy } E_\alpha^{(0)}}$

$\mathcal{H}'$ in new $|\beta\rangle$ basis $= \left(\begin{array}{c|cc} \Gamma & \cdot & \cdot \\ \hline \cdot & K & 0 \\ \cdot & 0 & K' \end{array}\right)$

←

$E_1 \approx E_1^{(0)} + \Gamma$

$E_2 \approx E_\alpha^{(0)} + K$

$E_3 = E_\alpha^{(0)} + K'$

$\Uparrow$

◐ Normaliz^{n}: $\underset{\text{FULL}}{|n\rangle} = \textcircled{1}\underbrace{|n^{(0)}\rangle}_{\substack{\text{UNPERTURBED}\\ \text{STATE ONLY}\\ \text{CONTRIBUTES HERE}}} + \varepsilon|n^{(1)}\rangle + \varepsilon^2|n^{(2)}\rangle + \ldots.$

● CHANGE of BASIS

■ Hwk 06,7 Assist ...

Given that

- matrix M that maps a vector onto a vector: $\vec{v} = M\vec{u}$
- transformation $\mathbb{R}$ from old to new basis: $\underset{\substack{\text{in}\\ \text{NEW}\\ \text{BASIS}}}{\vec{u}\,'} = \mathbb{R}\underset{\substack{\text{in}\\ \text{OLD}\\ \text{BASIS}}}{\vec{u}}$
- new orthonormal basis vectors, written in old orthonormal basis, are $\{\vec{e}_1, \vec{e}_2, \ldots\}$

THEN

$$\mathbb{R}^{-1} = \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix} \quad \& \quad \underset{\substack{\text{in}\\ \text{NEW}\\ \text{BASIS}}}{\mathbb{M}'} = \mathbb{R}\underset{\substack{\text{in}\\ \text{OLD}\\ \text{BASIS}}}{\mathbb{M}}\mathbb{R}^{-1}$$

VARIATIONAL PRINCIPLE

DISC 8

$$E_{gs} \leq \langle \hat{\mathcal{H}} \rangle_{\psi_{trial}}$$

corollary: $$E_{1ex} \leq \langle \hat{\mathcal{H}} \rangle_{\underbrace{\psi_{trial} \perp \psi_{gs}}}$$

Usual case: $V(x)$ even
which ⇒ $\psi_{GS}(x)$ even
& $\psi_{1ex}(x)$ odd

- always include free parameters
- normalization is NOT a free parameter! calculate it FIRST
∵ usu depends on the other parameters
- 1D: $\psi_{trial} \sim e^{-x^2 A} \cdots$
3D: $\psi_{trial} \sim e^{-rB} \cdots$
usu. good choices

TIME-DEP HAMILTONIANS

- Usually, focused on TRANSITION PROBABILITIES $P_{i \to f}$

e-states of some relevant t-indep $\mathcal{H}_0$
e.g. $\mathcal{H}|_{t=0}$

SUDDEN / ADIABATIC APPROX

HWK 8,9

$[\psi \,/\, n]$ unchanged when $\Delta \mathcal{H}$ occurs over a time interval Δt $[\ll / \gg]$ T

↑ wavefn

↑ principal q.no.

TIME-DEP PT

DISC 9

SETUP

$$\mathcal{H}(t) = \mathcal{H}^{(0)} + \mathcal{H}'(t)$$

t-indep AND solvable $\{E_n^{(0)}, |n^{(0)}\rangle\}$

expand $$|\psi(t)\rangle = \sum_n \underbrace{c_n(t)\, e^{-i\omega_n t}}_{\text{t-dep amplitudes}} |n^{(0)}\rangle$$ ← unpert. basis

initial conditions $|\psi(t_0)\rangle = |i^{(0)}\rangle$

goal ⇒ $P_{i\to f} = |c_f(t)|^2$

Results summary

1: exact ODE's for $c_j(t)$

2: 1st order PT for $\mathcal{H}' \ll \mathcal{H}_0$

3: sinusoidal $\mathcal{H}'$ ⇔ FGR step-function

4: $\mathcal{H}'$ from E1 radiation

RESULT #1

DISC 10

{coupled ODEs} for exact $\{c_j(t)\}$

⇒ solvable usu. only for 2-state systems

EXACT: $$i\hbar\, \dot{c}_f(t) = \sum_n \mathcal{H}'_{fn}\, e^{i\omega_{fn} t}\, c_n(t)$$

transition matx elem $\mathcal{H}'_{fn}$

freq. ω_{fn}

RESULT #2 : $\mathcal{H}'(t) \ll \mathcal{H}_0 \to$ 1st-order $c_j^{(1)}(t)$ in perturbative expansion

DISC 9

… result #2': recursive relation for $c_n^{(j)}(t)$:

j^{th} order PT: $$i\hbar\, \dot{c}_f^{(j)}(t) = \sum_n \mathcal{H}'_{fn}(t)\, e^{i\omega_{fn} t}\, c_n^{(j-1)}(t)$$ ..... graphical represent^n

RESULT #3: Sinusoidal $\mathcal{H}'(t) \rightarrow \cdots \rightarrow$ F.G.R.

DISC 11: FGR deriv for step $\mathcal{H}'(t)$

- $$\mathcal{H}'(t) = V(\vec{r})e^{i\omega t} + V^*(\vec{r})e^{-i\omega t}$$

→ ∃ 2 resonances

$$C_f^{(1)}(t) = -\frac{1}{\hbar}\left[\frac{V_{fi}\,e^{i\Omega_+ t'}}{\Omega_+} + \frac{V_{fi}^*\,e^{i\Omega_- t'}}{\Omega_-}\right]_0^t$$

where $\boxed{\Omega_\pm \equiv \omega_{fi} \pm \omega}$ → reso @ $\Omega_+ = 0$, $\Omega_- = 0$

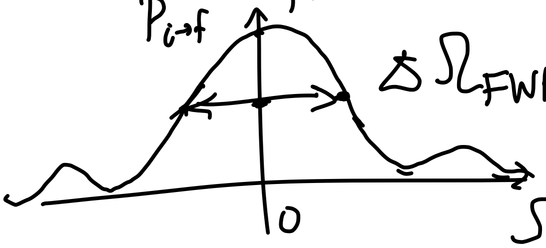
resonances: "absorption" & "stimulated emission" ←

→ key application: lasers

→ near 1 resonance

$$P_{i\to f}(t) \approx \frac{4|V_{fi}|^2}{\hbar^2}\left[\frac{\sin \Omega_\pm t/2}{\Omega_\pm t/2}\right]^2\left(\frac{t}{2}\right)^2$$

Ω-dep @ fixed t



$\Delta\Omega_{FWHM} \sim \frac{1}{t}$

$\Omega = \omega_{fi} + \omega$ OR $\omega_{fi} - \omega$ OR ω_{fi} for $\mathcal{H}'(t)$ = STEP case of DISC 11

t-dep on resonance (@ $\Omega_+ = 0$ OR $\Omega_- = 0$)

$$P_{i\to f} \approx \frac{|V_{fi}|^2}{\hbar^2}\,t^2$$

⇒ $t\to\infty$ on resonance gives F.G.R.

$$P_{i\to f} \xrightarrow[t\to\infty]{} \frac{4|V_{fi}|^2}{\hbar^2}\pi \cdot \delta(\Omega_\pm)\cdot\frac{t}{2}$$

∴ TRANSITION RATE $R_{i\to f} \equiv \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar^2}|V_{fi}|^2\delta(\Omega_\pm)$

↳ ∴ for a continuum of states: $W_{i\to f} \equiv R_{i\to\int f} = \frac{2\pi}{\hbar}|V_{fi}|^2 n(E_f)\Big|_{E_i\pm\hbar\omega}$

● RESULT #4 : E1 radiation

● DISC 12

▪ $V(\vec{r})_{E1} \approx -q\vec{E}_0\cdot\vec{r}$ when

- $\lambda_{\text{EM WAVE}} \ll r_{\text{system}}$
- $F_B \ll F_E$

show: true for MANY atomic situations

⇒ E1 selection rules:

$V_{fi} = -E_0\,{}_f\langle nlm|q\vec{r}|nlm\rangle_i$ = non-zero only when

transition matx elem

- $\Delta l = 0$

AND ● $\Delta m_l = 0, \pm 1$

● E1 photons can't flip spin

$\Delta S = 0$