Time Independent PT = Perturbation Theory

§6.1, 6.2

NON-DEGENERATE CASE

t-independent

setup: $\hat{H} = \hat{H}_0 + \hat{H}'$

BIG, "unperturbed" * EIGEN-SOLVABLE

small "perturbation", "$\hat{H}' \ll \hat{H}_0$"

*can find exact {e-values} & {e-states} of H_0

Techniques:

- ★ Dial of Explicit Smallness: ε
- ★ Equate separate orders of ε
- ★ PROJECT ONTO E-STATES: $\langle e_q|$
- ★ Hermiticity of $\hat{H}$ … & $\hat{H}_0, \hat{H}'$:

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

MOVE   no change

Setup: Dial of Explicit Smallness

$$\hat{H} = \hat{H}_0 + \varepsilon \hat{H}'$$

dimensionless $\varepsilon \ll 1$ … allows us to keep track of orders of smallness

Goal: Find e-things of $\hat{H}$ as a power series in ε:

$$\left.\begin{aligned} E_n &= E_n^{(0)} + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)} + \cdots \\ |n\rangle &= |n^{(0)}\rangle + \varepsilon |n^{(1)}\rangle + \varepsilon^2 |n^{(2)}\rangle + \cdots \end{aligned}\right\}$$

plug this form into eigen-equation $\hat{H}|n\rangle = E_n|n\rangle$

known: e-things of unperturbed $\hat{H}_0$

Plug: $[\hat{\mathcal{H}} - E_n]\,|n\rangle = 0 \Leftarrow$ eigen-equation

$$0 = [\hat{\mathcal{H}}_0 + \varepsilon \hat{\mathcal{H}}' - E_n^{(0)} - \varepsilon E_n^{(1)} - \mathcal{O}(\varepsilon^2) \ldots]$$
$$\times [|n^{(0)}\rangle + \varepsilon |n^{(1)}\rangle + \mathcal{O}(\varepsilon^2) \ldots]$$

Equate by order of ε!

Order $\boxed{\varepsilon^{(0)}}$: $\boxed{\hat{\mathcal{H}}_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle}$ part of our setup

WANT WANT

Order $\boxed{\varepsilon^{(1)}}$: $(\hat{\mathcal{H}}_0 - E_n^{(0)}) \cdot \cancel{\varepsilon} \underline{\underline{|n^{(1)}\rangle}} + \cancel{\varepsilon} (\hat{\mathcal{H}}' - \underline{\underline{E_n^{(1)}}}) |n^{(0)}\rangle = \emptyset$

Project onto UNPERTURBED e-states:

Hit equation from left with $\langle m^{(0)}|$

going to write $|n^{(1)}\rangle = a_1 |1^{(0)}\rangle + a_2 |2^{(0)}\rangle + \cdots$ as linear comb. of unperturbed states = basis that we HAVE

$$\emptyset = \underbrace{\langle m^{(0)} | \hat{\mathcal{H}}_0 \underline{\underline{n^{(1)}}}\rangle}_{E_m^{(0)} \langle m^{(0)} | \underline{\underline{n^{(1)}}}\rangle} - E_n^{(0)} \langle m^{(0)} | \underline{\underline{n^{(1)}}}\rangle + \langle m^{(0)} | \hat{\mathcal{H}}' | n^{(0)}\rangle - \underline{\underline{E_n^{(1)}}} \underbrace{\langle m^{(0)} | n^{(0)}\rangle}_{\delta_{mn}}$$

MOVE

1st order

$$\boxed{(E_n^{(0)} - E_m^{(0)}) \langle m^{(0)} | \underline{\underline{n^{(1)}}}\rangle = \langle m^{(0)} | \hat{\mathcal{H}}' | n^{(0)}\rangle - \underline{\underline{E_n^{(1)}}} \delta_{mn}}$$

WANT WANT

case $m=n$: get $E_n^{(1)}$ ∵ zaps LHS!

$$\boxed{E_n^{(1)} = \langle n^{(0)} | \hat{\mathcal{H}}' | n^{(0)} \rangle = \mathcal{H}'_{nn}}$$

nth diagonal matrix element of perturbation op $\hat{\mathcal{H}}'$

→ ⊕ 1st order energy correction for nth state is just EXPECTATION VALUE of $\mathcal{H}'$ in nth state

case $m \neq n$: get $|n^{(1)}\rangle$

$$\boxed{\langle m^{(0)} | n^{(1)} \rangle = \frac{\langle m^{(0)} | \hat{\mathcal{H}}' | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} = \frac{\mathcal{H}'_{mn}}{E_n^{(0)} - E_m^{(0)}}}$$

Build $\boxed{|n^{(1)}\rangle = \sum_{m \neq n} |m^{(0)}\rangle \frac{\mathcal{H}'_{mn}}{E_n^{(0)} - E_m^{(0)}}}$

→ ⊕ only applies for $m \neq n$ ... we have NO info on $\langle n^{(0)} | n^{(1)} \rangle$ ...

⊘ **NORMALIZATION** of $|n^{(0)}\rangle$ contribution to $|n\rangle$

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

e-state of $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$

NORMALIZ^{n} CONVENTION

only appearance of $|n^{(0)}\rangle$

only contains $|m^{(0)}\rangle$ terms with $m \neq n$

$$L = \sqrt{(10^5 m)^2 + (2m)^2}$$
$$= 10^5 m \sqrt{1 + (2\times 10^{-5})^2}$$
$$\approx 10^5 m \left[1 + \tfrac{1}{2}(2\times10^{-5})^2\right]$$
$$= 10^5 m \left[1 + \underset{\approx\approx\approx}{2\times10^{-10}}\right]$$

exactly analogous to normalization (= size) calculation for a QM state:

$$|\psi\rangle = a\,|1s0\rangle + b\,|2s0\rangle + c\,|2p{+}1\rangle + d\,|2p0\rangle + \cdots$$

nlm

orthonormal basis

$\therefore$ magnitude^2 $\langle\psi|\psi\rangle$

$= $ Pythagoras

$= a^2 + b^2 + c^2 + \cdots$

$= 1$ SET TO

normaliz$\underline{^n}$ condition

$$\vec{L} = 10^5 m\,\hat{x} + 2m\,\hat{y}$$

orthonorm. basis

$$|\vec{L}|^2 = (10^5 m)^2 + (2m)^2$$
$$= \vec{L}\cdot\vec{L} = \langle \vec{L}|\vec{L}\rangle$$
$$= (10^5 m\,\hat{x} + 2m\,\hat{y})\cdot(10^5 m\,\hat{x} + 2m\,\hat{y})$$
$$= (10^5 m)^2 + (2m)^2 + \text{NO } \cancel{\hat{x}\cdot\hat{y} \text{ terms}}$$

$\because \hat{x}\perp\hat{y}$

Perturbation series:

STOP HERE for $\underline{\text{1st order}}$ calc$\underline{^n}$

$$|n\rangle = 1\,|n^{(0)}\rangle + \sum_{m\neq n} |m^{(0)}\rangle\left[\mathcal{O}(\varepsilon) + \cdots\right]$$

$$\therefore \langle n|n\rangle = 1^2 + \sum_{m\neq n}\left[\mathcal{O}(\varepsilon)\right]^2 > 1$$

CONVENTION

but norm$\underline{^n}$ error is $\underline{\underline{\text{2nd order}}}$

Higher order PT (still non-degenerate)

Eigen-equation was:

$$\emptyset = \Big[\underbrace{\mathcal{H}_0 + \varepsilon \mathcal{H}'}_{\mathcal{H}} - \underbrace{\sum_{j=0}^{\infty} \varepsilon^j E_n^{(j)}}_{E_n}\Big] \times \underbrace{\Big[\sum_{k=0}^{\infty} \varepsilon^k |n^{(k)}\rangle\Big]}_{|n\rangle}$$

$$[\ \mathcal{H} \quad - \quad E_n\ ] \times |n\rangle$$

Terms of order ε^i for $i \geq 2$:

$$(\mathcal{H}_0 - E_n^{(0)})|n^{(i)}\rangle + (\mathcal{H}' - E_n^{(1)})|n^{(i-1)}\rangle = \sum_{k=0}^{i-2} E_n^{(i-k)} |n^{(k)}\rangle$$

ORDER $\boxed{i=2}$ hit with $\langle m^{(0)}|$ from left:

$$\underbrace{(E_m^{(0)} - E_n^{(0)})}_{\text{ZERO}} \underbrace{\langle m^{(0)}|n^{(2)}\rangle}_{\text{WANT}} + \langle m^{(0)}|\mathcal{H}' - \underbrace{E_n^{(1)}}_{\text{KNOW}}|\underbrace{n^{(1)}}_{\text{KNOW}}\rangle = \underbrace{E_n^{(2)}}_{\text{WANT}} \underbrace{\langle m^{(0)}|n^{(0)}\rangle}_{\delta_{mn}}$$

case $m=n$

$$E_n^{(2)} = \langle n^{(0)}|\hat{\mathcal{H}}' - E_n^{(1)}|n^{(1)}\rangle$$

$$= \langle n^{(0)}|\mathcal{H}'|n^{(1)}\rangle - E_n^{(1)} \underbrace{\langle n^{(0)}|n^{(1)}\rangle}_{\text{ZERO because of our normaliz}^n\text{ convention}}$$

generalizes easily to $i>2$

$$\boxed{E_n^{(j)} = \langle n^{(0)}|\mathcal{H}'|n^{(j-1)}\rangle}$$

Degenerate PT

Return to $\mathcal{O}(\varepsilon^1)$ equation:

1st order $\mathcal{O}(\varepsilon^1)$

$$\boxed{(E_n^{(0)}-E_m^{(0)})\langle m^{(0)}|\underline{n^{(1)}}\rangle = \langle m^{(0)}|\hat{\mathcal{H}}'|n^{(0)}\rangle - \underline{E_n^{(1)}}\delta_{mn}}$$

case $m=n$: $E_n^{(1)} = \mathcal{H}'_{nn}$ in unperturbed basis $\{|n^{(0)}\rangle\}$

case $m\neq n$: $\langle m^{(0)}|n^{(1)}\rangle = \mathcal{H}'_{mn}/(E_n^{(0)}-E_m^{(0)})$

↑ PROBLEM!

IF $E_n^{(0)} = E_m^{(0)}$ ie. if $m \,\&\, n$ states are DEGENERATE @ unperturbed level

For degenerate states$^{(0)}$

$m = \alpha_1$, $n = \alpha_2$ with $E_\alpha \equiv E_{\alpha_1} = E_{\alpha_2} = \cdots$ & maybe more in $\{\alpha_1, \alpha_2, \cdots\}$: DEGEN SUBSPACE

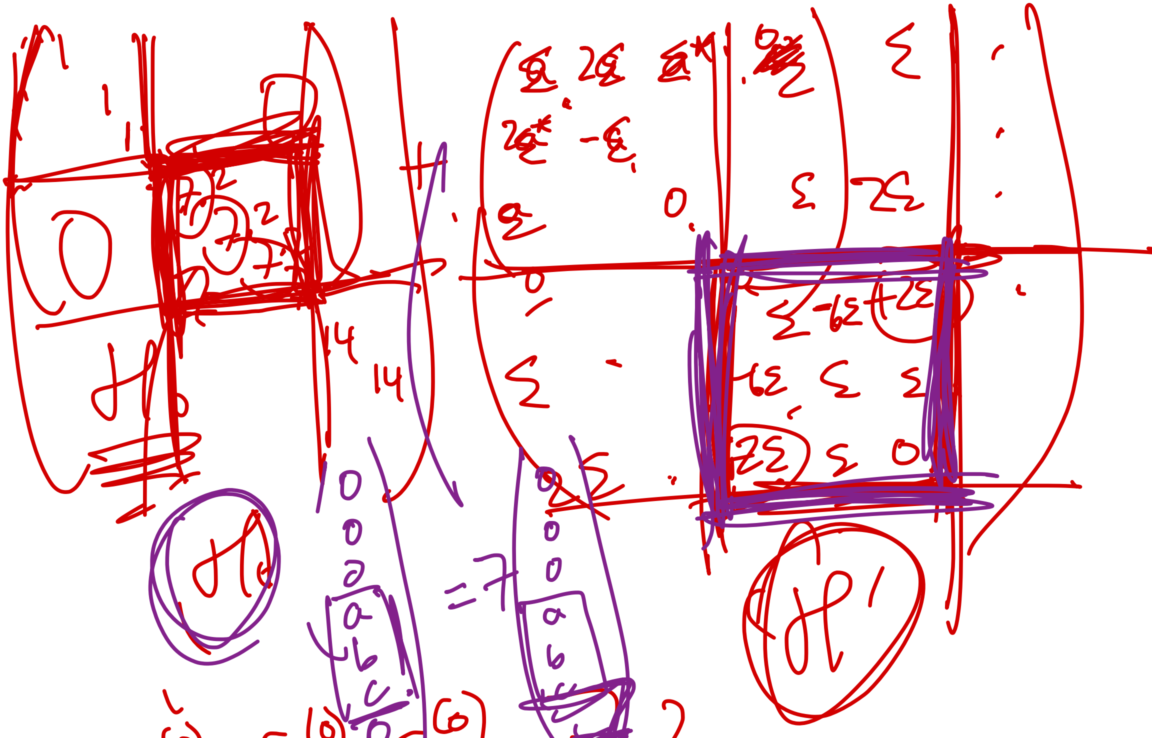
$$\underbrace{(E_{\alpha_1}^{(0)}-E_{\alpha_2}^{(0)})}_{\text{(ZERO)}}\langle \alpha_1^{(0)}|\alpha_2^{(1)}\rangle = \langle \alpha_1^{(0)}|\mathcal{H}'|\alpha_2^{(0)}\rangle - E_{\alpha_1}^{(1)}\cancelto{0}{\delta_{\alpha_1\alpha_2}}$$

$\therefore$ $\boxed{\text{MUST HAVE } \langle \alpha_i^{(0)}|\mathcal{H}'|\alpha_j^{(0)}\rangle = \emptyset \text{ with } i\neq j}$

for any two states α_i, α_j in a degenerate subspace

ie. perturbation matrix $\mathcal{H}'$ must be diagonal within any degenerate subs ace $\mathbf{D} \equiv \{|\alpha_i\rangle\}$

➡ change to a basis $\mathbf{D} = \{|\beta_1\rangle, |\beta_2\rangle, \cdots\}$ that diagonalizes $\mathcal{H}'$ within subspace $\mathbf{D}$



$$E_4^{(0)} = E_5^{(0)} = E_6^{(0)} = 7$$

$$D = \left\{ \begin{pmatrix}0\\0\\0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix} \right\} = \{|\alpha_i\rangle\}$$

FIND

$$D = \{|\beta_i\rangle\} = \left\{ \begin{pmatrix}0\\0\\0\\a\\b\\c\end{pmatrix}, \begin{pmatrix}0\\0\\0\\d\\e\\f\end{pmatrix}, \begin{pmatrix}0\\0\\0\\g\\h\\i\end{pmatrix} \right\}$$

$\Rightarrow H'$ is diagonal using these ex.1 2-state system, matrix representation

$$\underset{\text{FULL}}{\mathcal{H}} = \begin{pmatrix} 1 & a \\ a & 2 \end{pmatrix} \quad \text{with } \underline{a \ll 1}$$

$$\underset{\text{perturbative approach}}{=} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}}_{\text{BIG } \mathcal{H}_0} + \underbrace{\begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}}_{\text{small } \mathcal{H}'}$$

Steps: for non-degen PT

① Find e-things $\{|n^{(0)}\rangle\}$ & $\{E^{(0)}\}$ of unperturbed $\mathcal{H}_0$

i.e. diagonalize $\mathcal{H}_0$

② find $\{E_n^{(1)}\}$

③ find $\{|n^{(1)}\rangle\}$

④ find $\{E_n^{(2)}\}$

.....

① $\mathcal{H}_0$ is ALREADY DIAGONAL

$\therefore$ e-states $= \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ & $\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \{|n^{(0)}\rangle\}$

& e-values $= 1$ & $2 = \{E_n^{(0)}\}$

② Find $E_n^{(1)} = \langle n^{(0)}|\mathcal{H}'|n^{(0)}\rangle = \mathcal{H}'_{nn} = \underbrace{\langle \mathcal{H}' \rangle_{\text{in } n^{(0)} \text{ state}}}^{\text{expec value of } \mathcal{H}'}$

$= \emptyset$ for both states

No 1st-order energy corrections $(@\,\mathcal{O}(a^1))$

④ Find $E_n^{(2)} = \sum_{m \neq n} \dfrac{|\mathcal{H}'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}} = \begin{cases} \text{for } n=1: & \dfrac{|\mathcal{H}'_{21}|^2}{E_1^{(0)} - E_2^{(0)}} = -a^2 = E_1^{(2)} \\ \text{for } n=2: & \dfrac{|\mathcal{H}'_{12}|^2}{E_2^{(0)} - E_1^{(0)}} = a^2 = E_2^{(2)} \end{cases}$

$\therefore$ Eigen-energies up to 2nd order PT are: $E_1 \approx 1 - a^2$ & $E_2 \approx 2 + a^2$

Take $a = 0.1 \rightarrow E_1 \approx 0.99$ & $E_2 \approx 2.01$

To Wolfram α! EXACT e-values for $\mathcal{H} = \begin{pmatrix} 1 & a \\ a & 2 \end{pmatrix}$ with $a = 0.1$

$E_1 = 0.990098 = 1 - 0.01 + 10^{-4} - 2\times10^{-6} = 1 - a^2 + a^4 - 2a^6 \ldots$

$E_2 = 2.0099 = 2 + 0.01 - 10^{-4} = \underbrace{2 + a^2}_{} - a^4 \ldots$

✓ match PT to $\mathcal{O}(a) + \mathcal{O}(a^2)$

ex 2 $\mathcal{H} = \begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix} \rightarrow \mathcal{H}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ & $\mathcal{H}' = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}$

with $a \ll 1$

now unperturbed e-values are DEGENERATE!

① $E_1^{(0)} = E_2^{(0)} = 1$ unperturbed

② 1st order: $E_n^{(1)} = \mathcal{H}'_{nn} = 0$ * still for both n=1,2

③ 2nd order: $E_n^{(2)} = \sum_{m \neq n} \dfrac{|\mathcal{H}'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$ divide by $\emptyset$ in denom!

problem with formalism @ 2nd order

EXACT e-values of $\begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix}$ with $a = 0.1$:

Wolfram α $E_1 = 0.9 = 1 - a$

$E_2 = 1.1 = 1 + \underbrace{a}_{}$

* 1st order correcⁿ NOT $\emptyset$!

Fix this using degenerate PT!

Here, degen. subspace $D = \{|\alpha_i^{(0)}\rangle\} = \left\{\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}\right\}$

is entire space

$\Rightarrow$ Find new basis $\{|\beta_i^{(0)}\rangle\}$ to replace that makes H' DIAGONAL within subspace D

diagonalize $\hat{H}' = \begin{pmatrix}0 & a\\a & 0\end{pmatrix}$

change H' to this basis

- Find e-vectors: $\left\{\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \text{ \& } \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}\right\} \equiv \{|\beta_i^{(0)}\rangle\}$

- H_0 doesn't change $\because$ a linear combination $|\beta^{(0)}\rangle$ of degenerate e-vectors $|\alpha_i^{(0)}\rangle$ is STILL a degenerate e-vector, with same e-value

- Transform $\hat{H}'$ to new basis $\{|\beta\rangle\}$

$$\hat{H}'_\beta = (R^{-1})^{*T}\hat{H}'R^{-1}$$

$$\vec{\psi}_\beta = R\,\vec{\psi}$$

NEW BASIS — OLD BASIS

where R transforms vectors from old $\rightarrow$ new basis

MATH PART: BASIS CHANGE

In general: define basis-change transformation matrix $\mathbb{R}$

$\Rightarrow$ new basis is $\{\vec{e}_1, \vec{e}_2, \ldots\}$: $\boxed{\underset{\text{in new basis}}{\vec{V}'} = \mathbb{R}\vec{V}}$

defin$^{\underline{n}}$ of VECTOR XFORM $\mathbb{R}$

(old basis is $\left\{\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}, \begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}, \ldots\right\}$)

then $\boxed{\mathbb{R}^{-1} = \begin{pmatrix} | & | & | & \\ e_1 & e_2 & e_3 & \cdots \\ | & | & | & \end{pmatrix}}$

why?

$\underset{\text{OLD BASIS}}{\vec{V}} = \mathbb{R}^{-1} \underset{\text{NEW BASIS}}{\vec{V}'}$ ... feed $\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}$ into $\mathbb{R}^{-1}$; pulls out 1st column of $\mathbb{R}^{-1}$:

$$\underbrace{\mathbb{R}^{-1}\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}}_{\text{this is } \vec{e}_1 \text{ written in NEW BASIS}} = \underbrace{\vec{e}_1}_{\text{written in OLD basis, which we know!}} = 1\text{st column of } \mathbb{R}^{-1}$$

Finally, how to transform a MATRIX to the new BASIS?

call it $\mathbb{M}$

$$\boxed{\vec{u} = \mathbb{M}\vec{v}} \ldots$$

both vectors in same basis

in new (PRIME) basis, must have $\vec{u}' = \mathbb{M}'\vec{v}'$

WANT a formula for this

Apply VECTOR TRANSFORM:

$$\left.\begin{aligned} \vec{u}' &= \mathbb{R}\vec{u} \\ \vec{v}' &= \mathbb{R}\vec{v} \end{aligned}\right\} \rightarrow (\mathbb{R}\vec{u}) = \mathbb{M}'(\mathbb{R}\vec{v})$$

HIT that on the LEFT with $\mathbb{R}^{-1}$: $\underbrace{\mathbb{R}^{-1}(\mathbb{R}}_{\mathbb{1}}\vec{u}) = \underbrace{\mathbb{R}^{-1}\mathbb{M}'(\mathbb{R}}\vec{v})$

$\mathbb{M}$ by comparison with $*$:

$$\vec{u} = \overbrace{(\mathbb{R}^{-1}\mathbb{M}'\mathbb{R})}\vec{v}$$

$$\therefore \mathbb{M} = \mathbb{R}^{-1}\mathbb{M}'\mathbb{R} \xrightarrow{\text{clearly}} \longrightarrow \longrightarrow \boxed{\mathbb{M}' = \mathbb{R}\mathbb{M}\mathbb{R}^{-1}}$$

OR hit with $\mathbb{R}^{-1}$ from right & $\mathbb{R}$ from left

$$\mathbb{R}^{-1} = \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix} \quad \therefore \mathbb{R} = \begin{pmatrix} ? \end{pmatrix}$$

and $\{\vec{e}_1, \vec{e}_2, \cdots\}$ form a new basis

= orthonormal set of unit vectors

determined by INNER PRODUCT

real 3D vectors

$$\langle \vec{e}_1 | \vec{e}_2 \rangle = \vec{e}_1 \cdot \vec{e}_2$$
$$= \vec{e}_1^{\,T} \vec{e}_2$$

$\therefore$ orthonormal set $\{\vec{e}_i\}$ has

$$\boxed{\vec{e}_i^{\,T} \vec{e}_j = \delta_{ij}}$$

If $\mathbb{R}^{-1} = \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix}$

real 3D vectors

then $\boxed{\mathbb{R} = (\mathbb{R}^{-1})^T = \begin{pmatrix} — e_1 — \\ — e_2 — \\ \vdots \end{pmatrix}}$

$$\begin{pmatrix} — e_1 — \\ — e_2 — \\ \vdots \end{pmatrix} \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix} = \delta_{ij} = \mathbb{1}$$

QM Hilbert space

$$\langle \vec{e}_1 | \vec{e}_2 \rangle = \vec{e}_1^{\,\dagger} \vec{e}_2$$
$$= \vec{e}_1^{\,T*} \vec{e}_2$$

$\therefore$ orthonormal set $\{\vec{e}_i\}$

has $\boxed{\vec{e}_i^{\,T*} \vec{e}_j = \delta_{ij}}$

If $\mathbb{R}^{-1} = \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix}$

QM Hilbert space

then $\boxed{\mathbb{R} = (\mathbb{R}^{-1})^\dagger = (\mathbb{R}^{-1})^{T*} = \begin{pmatrix} — e_1^* — \\ — e_2^* — \\ \cdots \end{pmatrix}}$

$$\begin{pmatrix} — e_1^* — \\ — e_2^* — \\ \vdots \end{pmatrix} \begin{pmatrix} | & | & \\ e_1 & e_2 & \cdots \\ | & | & \end{pmatrix} = \delta_{ij} = \mathbb{1}$$

$\therefore \mathbb{R}^{-1} = \mathbb{R}^T$

$\mathbb{M}' = \mathbb{R}\,\mathbb{M}\,\mathbb{R}^T$

$\therefore \mathbb{R}^{-1} = \mathbb{R}^\dagger = \mathbb{R}^{T*}$

$\mathbb{M}' = \mathbb{R}\,\mathbb{M}\,\mathbb{R}^{-1}$
$= \mathbb{R}\,\mathbb{M}\,\mathbb{R}^\dagger$

Back to our example:

degen subspace $\mathbb{D} = \left\{ \begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix} \right\}_{|\alpha\rangle} = \left\{ \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \right\}_{|\beta\rangle}$

OLD BASIS

NEW BASIS that diagonalizes $\mathcal{H}' = \begin{pmatrix}0 & a\\ a & 0\end{pmatrix}$ OLD BASIS

Try it: what is $\mathcal{H}'$ in new basis $|\beta\rangle$?

$$\underbrace{\mathcal{H}'_\beta}_{\text{NEW BASIS}} = \mathbb{R}\,\mathcal{H}'\,\mathbb{R}^{-1} \quad \text{where } \mathbb{R}^{-1} = \begin{pmatrix} | & | \\ \beta_1 & \beta_2 \\ | & | \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$\mathbb{R} = \mathbb{R}^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & a\\ a & 0\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}a & -a\\ a & a\end{pmatrix} = \frac{1}{2}\begin{pmatrix}2a & 0\\ 0 & -2a\end{pmatrix} = \begin{pmatrix}a & 0\\ 0 & -a\end{pmatrix}^{*}$$

it's diagonal ✓ ← NEW-BASIS PERTURBATION

$\therefore$ PT for eigen-energies of $\mathcal{H} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}}_{\text{OLD BASIS}}$:

$$E_1^{(0)} + E_1^{(1)} = 1 + \left(\mathcal{H}'_{11}\right)^{*}_{\text{NEW BASIS } \beta} = 1 + a$$

$$E_2^{(0)} + E_2^{(1)} = 1 + \left(\mathcal{H}'_{22}\right)^{*}_{\text{NEW BASIS } \beta} = 1 - a$$

✓ matches exact result

More math comments:

- Our derivation of $\vec{v}' = \mathbb{R}\vec{v} \Rightarrow \mathbb{M}' = \mathbb{R}\,\mathbb{M}\,\mathbb{R}^{-1}$ was based on definition of "matrix" $\mathbb{M}$ as

$$\vec{u} = \mathbb{M}\,\vec{v}$$

i.e. turns a vector into another vector, where "vector" $\equiv$ something that transforms with $\mathbb{R}$

This transform^n property makes our "matrix" $\mathbb{M}$ a TENSOR

- λ SCALAR $\equiv$ invariant under $\mathbb{R}$
- $\vec{v}$ VECTOR $\equiv$ transforms with some $\mathbb{R}$
- $\mathbb{M}$ TENSOR $\equiv$ also has specific transform^n properties $\because$ VECTOR = TENSOR $\cdot$ VECTOR

VECTOR = TENSOR · VECTOR : other versions of this definition

$\boxed{\vec{u} = \mathbb{M}\,\vec{v}}$ ... take inner product of this equation with some other vector $\vec{w}$:

$\langle \vec{w} | \vec{u} \rangle = \boxed{\langle \vec{w} | \mathbb{M}\vec{v} \rangle = \text{SCALAR}}$ ∵ inner product always maps two elements (here VECTORS) onto a SCALAR

= INVARIANT under transform^{n} $\mathbb{R}$

alternate defining property of a tensor $\mathbb{M}$

3D vectors:

scalar $= \vec{w}^{T}\,\mathbb{M}\,\vec{v}$

QM Hilbert space:

scalar $= \vec{w}^{T*}\,\mathbb{M}\,\vec{v}$

"bilinear vector" constructions

e.g. 2KE $= \vec{\omega}^{T}\,\underset{\text{inertia}}{\mathbb{I}}\,\vec{\omega}$

e.g. scalar $= \vec{w}^{T}\,\mathbb{M}\,\vec{v}$ ... our tensor transform is $\mathbb{M}' = \mathbb{R}\mathbb{M}\mathbb{R}^{-1}$

rotate to new

rotates back to old

invariant scalar $= \underset{\text{new basis}}{\vec{w}'}\,\underbrace{\underset{\text{new basis}}{(\mathbb{M}')}}_{}\,\underset{\text{new basis}}{\vec{v}'} = \underset{\text{old basis}}{\vec{w}\,\mathbb{M}\,\vec{v}}$

$\mathbb{M}' = (\mathbb{R}\mathbb{M}\mathbb{R}^{-1})$

one more def^n of tensor $\mathbb{M}$ in terms of vectors

($\equiv$ things that xform with $\mathbb{R}$)

$\mathbb{M} = |u\rangle\langle v| =$ OUTER PRODUCT

DIRECT PRODUCT

$$= \vec{u}\,\vec{v}^{T} = \begin{pmatrix} | \\ \vec{u} \\ | \end{pmatrix} \begin{pmatrix} \text{---} \ \vec{v} \ \text{---} \end{pmatrix} = \begin{pmatrix} u_1 v_1 & u_1 v_2 & \vdots \\ u_2 v_1 & \vdots & \vdots \\ \vdots & \vdots & \end{pmatrix}$$

3D vectors

$$= \vec{u}\,\vec{v}^{T*}$$

QM Hilbert space

Can also derive

$$\mathbb{M}' = \mathbb{R}\,\mathbb{M}\,\mathbb{R}^{-1}$$

from this definition of $\mathbb{M}$

$$\underline{\underline{\hat{H}}}\,\underline{\underline{\vec{e}_\lambda}} = \underline{\underline{\lambda}}\,\vec{e}_\lambda \Longrightarrow \underline{\underline{(\hat{H} - \lambda)}}\,\underline{\underline{\vec{e}_\lambda}} = \emptyset$$

$$(\hat{H} - \lambda\hat{1})\vec{e}_\lambda = 0 \Rightarrow$$

$$a e_1 + b e_2 + c e_3 = 0$$
$$d e_1 + e e_2 + f e_3 = 0$$
$$\cancel{g e_1 + h e_2 + i e_3 = 0}$$

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = 0$$

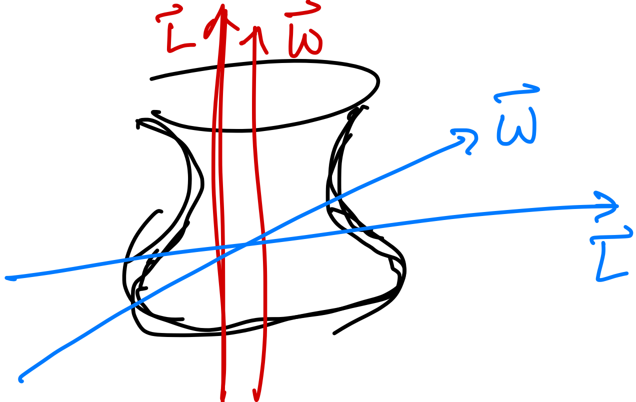
$$\Rightarrow \det\left|\hat{H} - \lambda\hat{1}\right| = 0$$

$\Rightarrow$ find λ's = e-values

$\Rightarrow$ go back to $(\hat{H} - \lambda\hat{1})\vec{e}_\lambda = 0$

& solve for these e-vectors

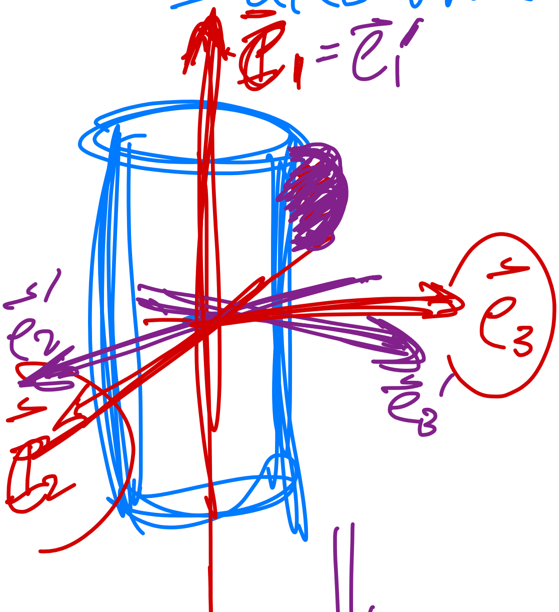
$\vec{L} = \overline{\overline{I}}\,\vec{\omega}$



e-vectors

$\equiv$ "principal axes" of rotation

$\equiv$ axes where $\vec{\omega} \parallel \vec{L}$



$\overline{\overline{I}}^{0}$ in $\{\vec{e}_i\}$ basis

$$= \begin{pmatrix} I_1 & & 0 \\ & I_{2=3} & \\ 0 & & I_{2=3} \end{pmatrix}$$

with $\{I_i\}$ e-values

$\Downarrow$

$$\underset{\text{SAME}}{\overline{\overline{I}}'} = \begin{pmatrix} I_1 & \varepsilon & -\varepsilon \\ \varepsilon & I_{2=3=2'=3'} + \varepsilon & \\ \varepsilon & & I_{2=3=2'=3'} \end{pmatrix} = \overline{\overline{I}}^{s.p.} = \overline{\overline{I}}^{0}$$

$= (\; + \varepsilon \overline{\overline{I}}'$

$$|\vec{V}\rangle = \begin{pmatrix} a \\ b \\ c \\ \vdots \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + c\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

$$= a|\vec{e}_1\rangle + b|\vec{e}_2\rangle + \cdots$$

$$+ \quad ?$$

$$|\vec{g}\rangle = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \vdots \end{pmatrix} = \alpha|\vec{e}_1'\rangle + \beta|\vec{e}_2'\rangle +$$

$$\neq (a+\alpha)|e_1\rangle + (b+\beta)|???\rangle$$

or $|e_i'\rangle$