Today – finish eg. on harmonic oscillator
– start on degenerate perturbation theory.

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Eg. Harmonic Oscillator

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 , \qquad \text{Perturbation } V = -qEx$$

Find the 1st & 2nd order corrections to the eigenvalues $E_n$.

① Time-independent perturbation theory.
② $E_n = (n+\frac{1}{2})\hbar\omega$, $n \geq 0$ are all non-degenerate.

} Non-deg. perturbation theory.

For all $n$, $E_n^{(1)} = 0$

$$\langle n | \hat{x} | n \rangle = 0 \quad \text{for all } n \qquad (|n\rangle = \psi_n^0)$$

because the expectation value of odd operators vanishes for states with definite parity;
$\hat{x}$ is an odd operator;
All $\psi_n^0(x)$ have definite parity because $H_0$ obeys inversion symmetry and has no degeneracies.

We can also show this using $\hat{a}$ and $\hat{a}^+$ operators.

Note that
$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}$$
$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\,\hat{p}$$

$$\hat{a} + \hat{a}^+ = 2\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}$$
$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^+)$$

We will denote $|\psi_n^0\rangle$ as $|n\rangle$.

$$\langle n | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | \hat{a} + \hat{a}^+ | n \rangle$$
$|n-1\rangle$    $|n+1\rangle$

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$, $n \geq 1$
$\hat{a}|0\rangle = 0$
$\hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$= 0$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|V_{mn}|^2}{E_n^0 - E_m^0} = (qE)^2 \sum_{m \neq n} \frac{|\langle m | \hat{x} | n \rangle|^2}{(n-m)\hbar\omega}$$

$$\langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left( \langle m | \hat{a} | n \rangle + \langle m | \hat{a}^\dagger | n \rangle \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left( \langle m | \sqrt{n} \, | n-1 \rangle + \langle m | \sqrt{n+1} \, | n+1 \rangle \right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left( \sqrt{n} \, \delta_{m,n-1} + \sqrt{n+1} \, \delta_{m,n+1} \right)$$

$$E_n^{(2)} = \frac{(qE)^2}{\hbar\omega} \frac{\hbar}{2m\omega} \sum_{m \neq n} \frac{\left( \underbrace{\sqrt{n} \, \delta_{m,n-1}}_{\substack{\text{non-zero when } m = n-1 \\ n-m = 1}} + \underbrace{\sqrt{n+1} \, \delta_{m,n+1}}_{\substack{\text{non-zero when } m = n+1 \\ n-m = -1}} \right)^2}{(n-m)}$$

$n$ is fixed.
Summing over $m \neq n$.

$$= \frac{(qE)^2}{2m\omega^2} \left( \frac{(\sqrt{n})^2}{(1)} + \frac{(\sqrt{n+1})^2}{(-1)} \right)$$

$$= \frac{(qE)^2}{2m\omega^2} \left( n - (n+1) \right)$$

$$= -\frac{(qE)^2}{2m\omega^2}$$

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## Degenerate perturbation theory

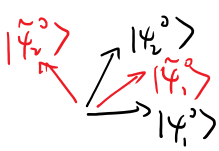
(A) For non-degenerate perturbation theory,

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{V_{mn}}{E_n^0 - E_m^0} |\psi_m^0\rangle \quad (\text{if } E_n^0 \neq E_m^0 \text{ for any } m)$$

If $E_n^0 = E_m^0$ for some $m$, $|\psi_n^1\rangle$ will blow up.

→ Suggests a problem with the zeroth order state.

(B) When there are degeneracies, eg. $E_1^0 = E_2^0$, $|\psi_1^0\rangle \neq |\psi_2^0\rangle$




$|\tilde{\psi}_1^0\rangle, |\tilde{\psi}_2^0\rangle$ : linear combinations of $\{|\psi_1^0\rangle, |\psi_2^0\rangle\}$ are also eigenstates with the same eigenvalue.

Non-degenerate perturbation theory.

$$E_n^1 = \langle \psi_n^0 | V | \psi_n^0 \rangle$$

But $\langle \psi_1^0 | V | \psi_1^0 \rangle$, $\langle \psi_2^0 | V | \psi_2^0 \rangle$, $\langle \tilde{\psi}_1^0 | V | \tilde{\psi}_1^0 \rangle$, $\langle \tilde{\psi}_2^0 | V | \tilde{\psi}_2^0 \rangle$

are not necessarily the same.

$\rightarrow$ Not well-defined.

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Q) What makes a good choice for the zeroth order state?

A) Choose the zeroth order states that connect smoothly to the perturbed state.

i.e. $|\psi_n(\lambda)\rangle = |\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots$

and $\longrightarrow |\psi_n^0\rangle$ as $\lambda \rightarrow 0$.

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Example to illustrate problem of the lack of smoothness in $|\psi(\lambda)\rangle$ if $|\psi^0\rangle$ is incorrectly chosen for the given $V$.

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad E_1^0 = E_2^0 = 1$$

$(1\ 0)V\begin{pmatrix}1\\0\end{pmatrix}$

$$V = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}$$

$(0\ 1)V\begin{pmatrix}0\\1\end{pmatrix}$

$$H(\lambda) = H_0 + V = \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix}$$

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Can actually find the eigenvalues of $H(\lambda)$ without perturbation theory:

Result is $H(\lambda)$ has eigenstates $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ with eigenvalue $1+\lambda$

$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$ —— " —— $1-\lambda$.

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If we use perturbation theory

Suppose we picked $|\psi_1^0\rangle \rightarrow \begin{pmatrix}1\\0\end{pmatrix}$, $|\psi_2^0\rangle \longrightarrow \begin{pmatrix}0\\1\end{pmatrix}$

and if we used $E_1^1 = \langle \psi_1^0 | V | \psi_1^0 \rangle$, then we get $E_n^1 = V_{11} = 0$

Similarly $E_2^1 = \langle \psi_2^0 | V | \psi_2^0 \rangle = 0$

} this gives the wrong result.

As you turn on $\lambda$ (from zero for $H = H_0$ to non-zero for $H(\lambda) = H_0 + V(\lambda)$), the state suddenly jumps from $\begin{pmatrix}1\\0\end{pmatrix}$ to $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ or $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$

or $\begin{pmatrix}0\\1\end{pmatrix}$

Smoothness condition for $|\psi(\lambda)\rangle$ fails.

Instead this is the correct procedure below.

$$H_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$V = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}$$

Diagonalize $V$ in the degenerate subspace.

In this case, ——— ∪ ——— is the whole Hilbert space.

So, Diagonalize $V = \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}$

$$\det(V - \mu I) = 0$$

$$\det \begin{pmatrix} -\mu & \lambda \\ \lambda & -\mu \end{pmatrix} = 0$$

$$\mu^2 - \lambda^2 = 0 \quad \Rightarrow \quad \mu = \pm\lambda$$

Find the eigenstates. $V\vec{e}_1 = \lambda \vec{e}_1$

$$\begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix} \quad \Rightarrow \quad x = y$$

So $\vec{e}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Similarly $\vec{e}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

In the basis of $\{\vec{e}_1, \vec{e}_2\}$, $V$ is $\begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}$.

So $E_1' = \lambda$

$E_2' = -\lambda$.

Energy to 1st order $E_1^0 + E_1' = 1 + \lambda$

$E_2^0 + E_2' = 1 - \lambda$. //

Q) Why is it that we have to diagonalize $V$ in the degenerate subspace for getting $E_n'$?

A) Go back to the expansions in $\lambda$.

Assumed smoothness in $\lambda$.

Compare coeff of $\lambda$:

$$H_0|\psi_n'\rangle + V|\psi_n^0\rangle = E_n^0|\psi_n'\rangle + E_n'|\psi_n^0\rangle \quad \text{— (1)}$$ from before.

Operate with $\langle \underbrace{\psi_{nd}^0}_{}|$ on both sides of (1).

Any state within the degenerate subspace with eigenvalue $E_n^0$.

i.e. $H_0|\psi_{nd}^0\rangle = E_n^0|\psi_{nd}^0\rangle$

$$\langle\psi_{nd}^0|H_0|\psi_n'\rangle + \langle\psi_{nd}^0|V|\psi_n^0\rangle = E_n^0\langle\psi_{nd}^0|\psi_n'\rangle + E_n'\langle\psi_{nd}^0|\psi_n^0\rangle.$$

Before $\langle \psi_n^0 | \psi_n^1 \rangle = 0$

but now, not necessarily so

$\therefore$ $|\psi_{nd}^0\rangle$ may not be $|\psi_n^0\rangle$.

$$\underbrace{E_n^0 \langle \psi_{nd}^0 | \psi_n^1 \rangle}_{\text{same}} + \langle \psi_{nd}^0 | V | \psi_n^0 \rangle = \underbrace{E_n^0 \langle \psi_{nd}^0 | \psi_n^1 \rangle}_{\text{same}} + E_n^1 \langle \psi_{nd}^0 | \psi_n^0 \rangle$$

$$\boxed{\langle \psi_{nd}^0 | V | \psi_n^0 \rangle = E_n^1 \langle \psi_{nd}^0 | \psi_n^0 \rangle} \quad \text{— (2)}$$