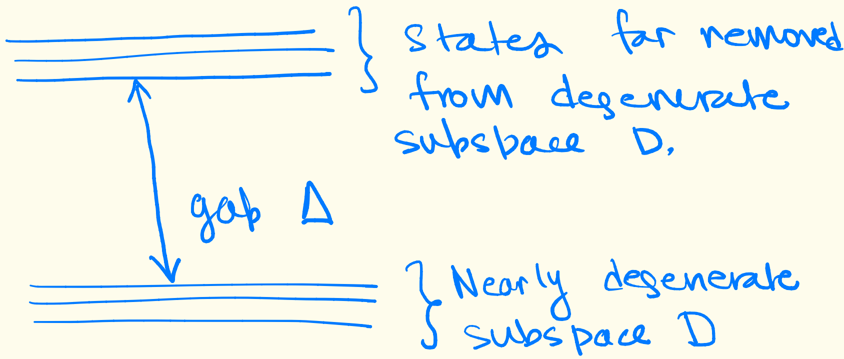
Degenerate State Perturbation Theory

As discussed above, perturbative corrections involve terms such as $\dfrac{\lambda \langle \alpha | H_1 | \beta \rangle}{E_\alpha - E_\beta}$,

and therefore naive perturbation theory breaks down if $\dfrac{\lambda \langle \alpha | H_1 | \beta \rangle}{E_\alpha - E_\beta} \gtrsim 1$.

For concreteness, consider the following spectrum for the unperturbed Hamiltonian H_0:



let's denote the states within the subspace D of interest as $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ etc. and those outside D as $|\mu\rangle, |\nu\rangle, |\lambda\rangle$ etc. (same notation as Gottfried-Yan).

Then, if $\dfrac{\lambda\langle\alpha|H_1|\beta\rangle}{E_\alpha - E_\beta} \gtrsim 1$ while

$\dfrac{\lambda\langle\alpha|H_1|\mu\rangle}{E_\mu - E_\alpha} \ll 1$, then one

expects that the perturbation λH_1 will significantly mix the states within D amongst each other while recieving only a small correction from states outside D.

Based on this expectation, let us write the perturbed eigenstates as

$$|a\rangle = \sum_{\alpha} c_\alpha |\alpha\rangle + \sum_{\mu} d_\mu |\mu\rangle$$

where $c_\alpha = O(1)$ and $d_\mu = O(\lambda)$.

Similar to the non-degenerate case, one can consider two different kinds of matrix elements of the Schrodinger's eqn. $\langle\beta|H|a\rangle = E_a\langle\beta|a\rangle = E_a c_\beta$ where $|\beta\rangle \in D$

and $\langle\nu|H|a\rangle = E_a\langle\nu|a\rangle = E_a d_\nu$

where $|\nu\rangle \notin D$.

Writing $H = H_0 + \lambda H_1$ and expanding these two equations after substituting $|a\rangle = \sum_\alpha c_\alpha |\alpha\rangle + \sum_\mu d_\mu |\mu\rangle$

the second equation becomes,

$$\langle \nu | \sum_\alpha \cancelto{0}{c_\alpha} \, \epsilon_\alpha |\alpha\rangle + \lambda \sum_\alpha c_\alpha \langle \nu | H_1 | \alpha \rangle$$

$$+ \langle \nu | \sum_\mu d_\mu \epsilon_\mu |\mu\rangle$$

$$+ \underbrace{\lambda \sum_\mu d_\mu \langle \nu | H_1 | \mu \rangle}_{O(\lambda^2)} = \epsilon_a d_\nu$$

Keeping terms only to $O(\lambda) \Rightarrow$

$$d_\nu = \frac{\lambda \sum_\alpha c_\alpha \langle \nu | H_1 | \alpha \rangle}{\epsilon_a - \epsilon_\nu}$$

To the leading order, ϵ_a = mean energy of levels within $D \equiv \epsilon_D$.

$$\Rightarrow \quad d_\nu = \lambda \sum_\alpha \frac{c_\alpha \langle \nu | H_1 | \alpha \rangle}{E_D - E_\nu} .$$

So far, c_α are still undetermined. To find them, let us consider the second equation above obtained by taking the dot product of the Schrodinger's eqn. with $\langle \beta | \in D$,

$$\langle \beta | \sum_\alpha c_\alpha E_\alpha | \alpha \rangle + \sum_\alpha \lambda \langle \beta | H_1 | \alpha \rangle c_\alpha + \sum_\nu \cancelto{0}{\langle \beta | d_\nu E_\nu | \nu \rangle} + \lambda \sum_\nu d_\nu \langle \beta | H_1 | \nu \rangle = E_a c_\beta$$

We now substitute the above obtained expression for d_ν in this eqn.

$$\Rightarrow \quad c_\beta E_\beta + \lambda \sum_\alpha \langle \beta | H_1 | \alpha \rangle c_\alpha + \lambda^2 \sum_\alpha c_\alpha \sum_\nu \frac{\langle \beta | H_1 | \nu \rangle \langle \nu | H_1 | \alpha \rangle}{\bar{E}_D - E_\nu}$$

$$= E_a c_\beta$$

This eqn. motivates one to define an "effective Hamiltonian" H_{eff} that acts only on the subspace D, and whose matrix elements are given by,

$$\langle \beta | H_{eff} | \alpha \rangle = \langle \beta | H_0 | \alpha \rangle + \lambda \langle \beta | H_1 | \alpha \rangle + \lambda^2 \sum_\nu \frac{\langle \beta | H_1 | \nu \rangle \langle \nu | H_1 | \alpha \rangle}{\bar{E}_D - E_\nu}$$

[Note: Compared to Gottfried-Yan, we have added a term $\langle \beta | H_0 | \alpha \rangle$ to $\langle \beta | H_{eff} | \alpha \rangle$. This is just a constant shift]

Then the above eqn. for coefficients c_α is nothing but the Schrodinger eqn for the eigenstates of H_{eff}.

To see this, we expand eigenstates of H_{eff} in the basis $\{|\alpha\rangle\}$ for D:

$|\psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle$. The Schrodinger eqn. is

$$H_{eff}|\psi\rangle = E_a|\psi\rangle$$

or

$$\sum_\alpha \langle\beta|H_{eff}|\alpha\rangle c_\alpha = E_a c_\beta$$

which is precisely the above eqn. for c_α [note that the term $\sum_\alpha \langle\beta|H_0|\alpha\rangle c_\alpha = \sum_\alpha c_\alpha \delta_{\alpha\beta} E_\alpha = E_\beta c_\beta$].

Therefore, we have reduced the degenerate perturbation theory to diagonalizing (i.e. finding eigenvectors and eigenvalues) of H_{eff}. Since the degenerate subspace for simple problems is typically small, this is a much simpler problem than diagonalizing the full Hamiltonian H. The outcome of this diagonalization will be the coefficients $\{c_\alpha\}$ (and in turn the coefficients $\{d_\nu\}$) which then determine the perturbed eigenstates to $O(\lambda)$, and eigenenergies to $O(\lambda^2)$.

A few illustrations of degenerate state perturbation theory

Example 1 : lets consider the following Hamiltonian :

$$H = -Z_1 Z_2 + h(X_1 + X_2)$$

$$[\equiv -Z_1 \otimes Z_2 + h(X_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes X_2)]$$

where $h \ll 1$. Therefore, we write

$H = H_0 + hH_1$ where $H_0 = -Z_1 Z_2$

and $H_1 = (X_1 + X_2)$.

The eigenspectrum of H_0 is

$E = +1$ $\underline{\qquad\qquad}$ $|01\rangle$ $\underline{\qquad\qquad}$ $|10\rangle$

$E = -1$ $\underline{\qquad\qquad}$ $|00\rangle$ $\underline{\qquad\qquad}$ $|11\rangle$ $\Big\}$ degenerate subspace D

If we are interested in how the perturbation hH_1 modifies the ground states of H_0, then we need to study the effective Hamiltonian H_{eff} within the degenerate subspace D spanned by $|00\rangle$ and $|11\rangle$. But before we do that, let's first find all the eigenstates and eigenvectors exactly for any h. This can be done because the problem has a finite-dimension Hilbert space. Since $[H, X_1X_2] = 0$, the eigenstates can be labelled by eigenvalues of the operator X_1X_2.

The subspace $X_1 X_2 = +1$ is spanned by the states $\frac{1}{\sqrt{2}}[|00\rangle + |11\rangle]$ and $\frac{1}{\sqrt{2}}[|01\rangle + |10\rangle]$, while the subspace $X_1 X_2 = -1$ is spanned by the states $\frac{1}{\sqrt{2}}[|00\rangle - |11\rangle]$ and $\frac{1}{\sqrt{2}}[|01\rangle - |10\rangle]$

where as usual $|0\rangle$ and $|1\rangle$ denote eigenstates of Z_i with eigenvalues $+1$ and -1 respectively.

Lets first consider the subspace $X_1 X_2 = +1$. The action of H within this subspace is:

$$H \frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]$$

$$= -\frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right] + \frac{2h}{\sqrt{2}}\left[|10\rangle + |01\rangle\right]$$

and

$$H \frac{1}{\sqrt{2}}\left[|10\rangle + |01\rangle\right]$$

$$= +\frac{1}{\sqrt{2}}\left[|10\rangle + |01\rangle\right] + \frac{2h}{\sqrt{2}}\left[|00\rangle + |11\rangle\right].$$

Therefore, within this subspace, H may be written as matrix,

$$H \equiv \begin{bmatrix} -1 & 2h \\ 2h & 1 \end{bmatrix}$$

The eigenvalues of H are

$\mp\sqrt{1+4h^2}$, and the corresponding

eigenvectors are $\cos(\theta/2)\left[\frac{|00\rangle+|11\rangle}{\sqrt{2}}\right]$

$+\sin(\theta/2)\left[\frac{|01\rangle+|10\rangle}{\sqrt{2}}\right]$, and

$$\sin(\theta/2)\left[\frac{|00\rangle+|11\rangle}{\sqrt{2}}\right]-\cos(\theta/2)\left[\frac{|01\rangle+|10\rangle}{\sqrt{2}}\right]$$

where $\tan(\theta)=-2h$.

Lets next find eigenvectors and eigenvalues within the subspace

$x_1 x_2 = -1$.

$$H \frac{1}{\sqrt{2}} [|00\rangle - |11\rangle]$$

$$= -\frac{1}{\sqrt{2}} [|00\rangle - |11\rangle]$$

$$+ \frac{h}{\sqrt{2}} [|10\rangle - |01\rangle + |01\rangle - |10\rangle]$$

$$= -\frac{1}{\sqrt{2}} [|00\rangle - |11\rangle]$$

$$H \frac{1}{\sqrt{2}} [|01\rangle - |10\rangle]$$

$$= +\frac{1}{\sqrt{2}} [|01\rangle - |10\rangle]$$

$$+ \frac{h}{\sqrt{2}} [|11\rangle - |00\rangle + |00\rangle - |11\rangle]$$

$$= \frac{1}{\sqrt{2}} [|01\rangle - |10\rangle].$$

Therefore, within this subspace, H may be written as matrix,

$$H \equiv \begin{bmatrix} -1 & \\ & 1 \end{bmatrix}$$

Therefore, the eigenvalues are ∓ 1 and the corresponding eigenvectors are $\dfrac{|00\rangle - |11\rangle}{\sqrt{2}}$ and $\dfrac{|01\rangle - |10\rangle}{\sqrt{2}}$, respectively.

Using these exact results, then the perturbed eigenstates and eigenvectors within the subspace D are :

$E = -1, \quad (|00\rangle - |11\rangle)/\sqrt{2}$

$E = -1 - 2h^2, \quad \dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$

Lets now derive this result using H_{eff} for the degenerate perturbation theory. Recall that the spectrum of H_0 is

$|01\rangle \qquad |10\rangle$

$\underbrace{|00\rangle \qquad |11\rangle}_{\text{degenerate subspace } D}$

Therefore, in our notation,

$$\{|\alpha\rangle\} = |00\rangle, \ |11\rangle$$

$$\{|\nu\rangle\} = |01\rangle, \ |10\rangle$$

$\langle 00 | H_{eff} | 00 \rangle$

$$= \langle 00 | H_0 | 00 \rangle + h \underbrace{\langle 00 | (x_1 + x_2) | 00 \rangle}_{\to 0}$$

$$+ h^2 \frac{\langle 00 | (x_1 + x_2) | 01 \rangle \langle 01 | (x_1 + x_2) | 00 \rangle}{-2 \; (= E_0 - E_D)}$$

$$+ h^2 \frac{\langle 00 | (x_1 + x_2) | 10 \rangle \langle 10 | (x_1 + x_2) | 00 \rangle}{-2}$$

$$= -1 - h^2$$

Similarly, $\langle 11 | H_{eff} | 11 \rangle = -1 - h^2$,

while $\langle 00 | H_{eff} | 11 \rangle$ is given

by,

$\langle 00 | H_{eff} | 11 \rangle$

$$= \langle 00 | \cancel{H_0} | 11 \rangle^{0} + h \langle 00 | \cancel{X_1 + X_2} | 11 \rangle^{0}$$

$$+ h^2 \frac{\langle 00 | (X_1 + X_2) | 01 \rangle \langle 01 | (X_1 + X_2) | 11 \rangle}{-2}$$

$$+ h^2 \frac{\langle 00 | (X_1 + X_2) | 10 \rangle \langle 10 | (X_1 + X_2) | 11 \rangle}{-2}$$

$$= -h^2$$

Therefore, as a matrix, H_{eff}

$$= \begin{bmatrix} -1 - h^2 & -h^2 \\ -h^2 & -1 - h^2 \end{bmatrix}$$

$$= (-1 - h^2) \mathbb{1} + -h^2 \tilde{X}$$

where $\tilde{X}$ acts within the degenerate subspace as

$\tilde{X}\,|00\rangle = |11\rangle$ and $\tilde{X}|11\rangle = |00\rangle$.

$\Rightarrow$ The eigenvectors and eigenvalues are :

$$E_1 = -1 - h^2 - h^2 = -1 - 2h^2$$

$$|E_1\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}},$$

and $E_2 = -1 - h^2 + h^2 = -1$

with $|E_2\rangle = \dfrac{|00\rangle - |11\rangle}{\sqrt{2}}$

which precisely matches the expression obtained above using exact calculation expanded to $O(h^2)$.