Higher-Order Perturbation Theory for a Degenerate Level

We have

$$H = H_0 + \lambda V \qquad 1$$

and g state $|m^a\rangle$ with the same energy when $\lambda = 0$

$$H_0 |m^0\rangle = E_D^0 |m^0\rangle \qquad 2$$

in which E_D^0 is the common energy of the g-dimensional space D spanned by the $|m^0\rangle$'s. We have assume that V completely lifts or breaks the degeneracy.

We know that the first task is to define the projection operator P_0 onto the space D

$$P_0 = \sum_{m \in D} |m^0\rangle\langle m^0| \qquad 3$$

and to diagonalize the $g \times g$ matrix

$$V_D = P_0 V P_0 \qquad 4$$

and find its e-vecs $|l^0\rangle$.

But let us follow Sakurai more closely.

Define P_1 as

$$P_1 = 1 - P_0 \,, \qquad 5$$

Is P_1 also a projection operator?

$$P_1^2 = (1-P_0)^2 = 1 + P_0^2 - 2P_0 = 1 + P_0 - 2P_0 = 1 - P_0$$
$$= P_1 \qquad 6$$

So, yes, P_1 is a projection operator.

We want to solve

$$0 = (E - H_0 - \lambda V)\,|\ell\rangle \qquad (7)$$

where $|\ell\rangle \to |\ell^0\rangle \in D$. We act on (7) with

$$I = P_0 + P_1 \qquad (8)$$

getting

$$0 = (E - H_0 - \lambda V)P_0|\ell\rangle + (E - H_0 - \lambda V)P_1|\ell\rangle \qquad (9)$$

or since $H_0 P_0 = E_D P_0$

$$0 = (E - E_D - \lambda V)P_0|\ell\rangle + (E - H_0 - \lambda V]P_1|\ell\rangle. \qquad (10)$$

We now use the projection operators P_0 and P_1 to split (10) into two equations.

Since $P_0(E-H_0)P_1 = 0$, we have

(5.2.3) $$0 = (E - E_D^0 - \lambda P_0 V) P_0 |l\rangle - \lambda P_0 V P_1 |l\rangle. \tag{11}$$

And since $P_1(E-E_D)P_0 = 0$, we get

(5.2.4) $$0 = -\lambda P_1 V P_0 |l\rangle + (E - H_0 - \lambda P_1 V) P_1 |l\rangle = 0 \tag{12}$$

since

$$[H_0, P_1] = [H_0, 1 - P_0] = -[H_0, P_0] = 0. \tag{13}$$

Now $P_1(E - H_0 - \lambda P_1 V P_1)$ is non-singular in the P_1 subspace because E is near E_D^0 and the evals of $P_1 H_0 P_1$ are not. So we can invert (12) getting

(5.2.5) $$P_1 |l\rangle = P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 |l\rangle. \tag{14}$$

So if

$$|l\rangle = |l^0\rangle + \lambda |l'\rangle + \dots \tag{15}$$

then

$$P_1 |l\rangle = P_1 (|l^0\rangle + \lambda |l'\rangle + \dots)$$

$$= \lambda P_1 |l'\rangle = P_1 \frac{\lambda}{E - H_0} P_1 V P_0 |l^0\rangle \tag{16}$$

or

$$P_1 |l'\rangle = \sum_{k \notin D} \frac{|k^0\rangle}{E_D^0 - E_k^0} \langle k^0 | V | l^0 \rangle \tag{17}$$

which we may write as

(5, 2, 6) $$P_1|\ell'\rangle = \sum_{k\notin D} \frac{|k^0\rangle}{E_D^0 - E_k^0} V_{k\ell}, \qquad (18)$$

Note that $V_{k\ell}$ connects state $|k^0\rangle \notin D$ to the state $|\ell^0\rangle \in D$.

To find $P_0|\ell\rangle$, we put (14) into (11)

$$0 = (E - E_D^0 - \lambda P_0 V) P_0|\ell\rangle - \lambda P_0 V P_1 \frac{\lambda}{E - H_0 - \lambda P_1 V P_1} P_1 V P_0 |\ell\rangle \qquad 19$$

or

$$0 = \left(E - E^0_D - \lambda P_0 V P_0 - \lambda^2 P_0 V P_1 \frac{1}{E - H_0 - \lambda V} P_1 V P_0\right) P_0|\ell\rangle . \qquad 20$$

To order λ, (20) is just

$$0 = (E - E^0_D - \lambda P_0 V P_0) P_0 |\ell\rangle . \qquad 21$$

The e-vals E are the roots of

$$0 = \det[E - E_D^0 - \lambda P_0 V P_0] = \det[E - E_D^0 - \lambda V_D] \qquad 22$$

and the e-vecs $|\ell^0\rangle$ solve

$$P_0 V P_0 |\ell^0\rangle = \Delta'_\ell |\ell^0\rangle \qquad (23)$$

or

$$\sum_{m \in D} \langle m'^0 | V | m^0 \rangle \langle m^0 | \ell^0 \rangle = \Delta'_\ell \langle m'^0 | \ell^0 \rangle . \quad (24)$$

Equations (21-24) are what we found in our notes on first-order perturbation theory

$$\Delta'_\ell = \langle \ell^0 | V_D | \ell^0 \rangle = \langle \ell^0 | V | \ell^0 \rangle . \quad 25$$

Now we approximate (20) as

(5.2.12) $$0 = \left(E - E_D^0 - \lambda P_0 V P_0 - \lambda^2 P_0 V P_1 \frac{1}{E_D^0 - H_0} P_1 V P_0 \right) P_0 | \ell \rangle . \quad 26$$

Suppose the e-vals of the $g \times g$ matrix $P_0 V P_0$ are v_i and the e-vecs are $P_0 | \ell_i^0 \rangle$

$$\left(P_0 V P_0 \right) P_0 | \ell^0_i \rangle = v_i \, P_0 | \ell^0_i \rangle . \quad 27$$

Then the e-vals of H to first order are

$$E_i^1 = E_D^0 + \lambda v_i . \quad 28$$

We assume that the g v_i are all different. So now we apply <u>non-degenerate</u> perturbation theory to (26) to find the correction $P_0 | \ell_i^1 \rangle$ in D to $P_0 | \ell_i^0 \rangle$.

We use (5.1.39)

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$$|n^1\rangle = \frac{\phi_n}{E_n^0 - \mathcal{H}_0} \mathcal{V} |n^0\rangle \tag{29}$$

with
$$\mathcal{V} = \lambda^2 P_0 V P_1 \frac{1}{E_D^0 - H_0} P_1 V P_0 \tag{30}$$

and
$$\phi_n = \sum_{j \neq i} |l_j^0\rangle\langle l_j^0| \tag{31}$$

and
$$\mathcal{H} = H_0 + \lambda P_0 V P_0 \tag{32}$$

to find
$$P_0 |l_i^1\rangle = \sum_{j \neq i} \frac{\lambda^2 P_0 |l_j^0\rangle\langle l_j^0| V P_1}{E_D^0 + \lambda v_i - E_D^0 - \lambda v_j} \frac{1}{E_D^0 - H_0} P_1 V |l_i^0\rangle \tag{33}$$

$$= \sum_{j \neq i} \frac{\lambda P_0 |l_j^0\rangle}{v_i - v_j} \langle l_j^0 | V P_1 \frac{1}{E_D^0 - H_0} P_1 V | l_i^0\rangle \tag{34}$$

$$= \sum_{j \neq i} \lambda \frac{P_0 |l_j^0\rangle}{v_i - v_j} \sum_{k \notin D} \langle l_j^0 | V | k^0\rangle \frac{1}{E_D^0 - E_k^0} \langle k^0 | V | l_i^0\rangle . \tag{35}$$

Now

$$|l\rangle = |l^0\rangle + \lambda P_1 |l^1\rangle + \lambda P_0 |l^1\rangle \qquad (36)$$

and since $P_0|l^1\rangle$ is of order λ, $\lambda P_0 |l^1\rangle$ is of order λ^2.

We choose

$$\langle l^0 | l\rangle = 1 \qquad (37)$$

and with

$$\Delta_l = \lambda \Delta_l^1 + \lambda^2 \Delta_l^2 + \cdots$$

$$= E_l - E_D^0$$

$$= \langle l^0 | \lambda V + H_0 - H_0 | l\rangle = \lambda \langle l^0 | V | l\rangle \qquad (38)$$

$$= \lambda \langle l^0 | V | l^0\rangle + \lambda^2 \langle l^0 | V | l^1\rangle + \cdots \qquad (39)$$

we see that

$$\Delta_l^2 = \langle l^0 | V | l^1\rangle$$

$$= \underbrace{\langle l^0 | V P_0 | l^1\rangle}_{\text{order } \lambda} + \langle l^0 | V P_1 | l^1\rangle \qquad (40)$$

So

$$\Delta_l^2 = \langle l^0 | V P_1 | l^1\rangle \qquad (41)$$

where by (17)

$$P_1|l^1\rangle = \sum_{k \notin D} \frac{|k^0\rangle\langle k^0|V|l^0\rangle}{E_D^0 - E_k^0} \tag{42}$$

so

$$\Delta_l^2 = \sum_{k \notin D} \frac{\langle l^0|V|k^0\rangle\langle k^0|V|l^0\rangle}{E_D^0 - E_k^0} \tag{43}$$

or

$$\Delta_l^2 = \sum_{k \notin D} \frac{|V_{kl}|^2}{E_D^0 - E_k^0} \ . \tag{44}$$