

(These notes combine treatment from Sakurai with the MIT OpenCourseWare [8.06 Quantum Physics III, Spring 2018](#), L1.1-L3.4).

Let H_0 be degenerate in the g -dimensional subspace D , whose eigenvalue is $E_D^{(0)}$. Since D is degenerate, we have some freedom to choose its set of orthonormal basis $\left\{ \left| d_i^{(0)} \right\rangle \right\}$. As we shall see later, the choice should be dictated by the requirement imposed by the degeneracy in various orders.

For perturbation strength λ , let the perturbed energy eigenvalue and eigenket corresponding to $\left| d_i^{(0)} \right\rangle$ be

$$E_{d_i}(\lambda) = E_D^{(0)} + \lambda \Delta_{d_i}^{(1)} + \lambda^2 \Delta_{d_i}^{(2)} + O(\lambda^3) \quad (1)$$

$$\left| d_i(\lambda) \right\rangle = \left| d_i^{(0)} \right\rangle + \lambda \left| d_i^{(1)} \right\rangle + \lambda^2 \left| d_i^{(2)} \right\rangle + O(\lambda^3) \quad (2)$$

In (1), we use subscript d_i to emphasize that the energy shift can be dependent on i .

Recall we will not try to normalize $\left| d_i \right\rangle$ until the very end, so in (2), we will maintain the coefficient for $\left| d_i^{(0)} \right\rangle$ as 1. Therefore we can conveniently assume that each of the higher order perturbation ket $\left| d_i^{(>0)} \right\rangle$ has no component along $\left| d_i^{(0)} \right\rangle$, i.e.,

$$\left\langle d_i^{(0)} \left| d_i^{(>0)} \right\rangle \right\rangle = 0 \quad (3)$$

because otherwise, we can absorb these components into the first term $\left| d_i^{(0)} \right\rangle$ and rescale (2).

The perturbed energy eigenequation is

$$(E_{d_i} - H_0) \left| d_i \right\rangle = \lambda V \left| d_i \right\rangle \quad (4)$$

Plug (1) and (2) into (4), we get

$$\begin{aligned} & \left[E_D^{(0)} + \lambda \Delta_{d_i}^{(1)} + \lambda^2 \Delta_{d_i}^{(2)} + O(\lambda^3) - H_0 \right] \left[\left| d_i^{(0)} \right\rangle + \lambda \left| d_i^{(1)} \right\rangle + \lambda^2 \left| d_i^{(2)} \right\rangle + O(\lambda^3) \right] \\ &= \lambda V \left[\left| d_i^{(0)} \right\rangle + \lambda \left| d_i^{(1)} \right\rangle + \lambda^2 \left| d_i^{(2)} \right\rangle + O(\lambda^3) \right] \end{aligned} \quad (5)$$

By matching different orders, we obtain a series of equations:

$$\lambda^0 \text{ order : } (E_D^{(0)} - H_0) \left| d_i^{(0)} \right\rangle = 0 \quad (6)$$

$$\lambda^1 \text{ order : } (E_D^{(0)} - H_0) \left| d_i^{(1)} \right\rangle + \Delta_{d_i}^{(1)} \left| d_i^{(0)} \right\rangle = V \left| d_i^{(0)} \right\rangle \quad (7)$$

$$\lambda^2 \text{ order : } (E_D^{(0)} - H_0) \left| d_i^{(2)} \right\rangle + \Delta_{d_i}^{(1)} \left| d_i^{(1)} \right\rangle + \Delta_{d_i}^{(2)} \left| d_i^{(0)} \right\rangle = V \left| d_i^{(1)} \right\rangle \quad (8)$$

(6) is just the unperturbed eigenequation.

For (7), we have two unknowns $\left| d_i^{(1)} \right\rangle$ and $\Delta_{d_i}^{(1)}$. But by left-applying $\left\langle d_j^{(0)} \right|$, we have

$$\begin{aligned} & \underbrace{\left\langle d_j^{(0)} \left| E_D^{(0)} - H_0 \right| d_i^{(1)} \right\rangle}_{=0} + \left\langle d_j^{(0)} \left| \Delta_{d_i}^{(1)} \right| d_i^{(0)} \right\rangle = \left\langle d_j^{(0)} \left| V \right| d_i^{(0)} \right\rangle \quad \Rightarrow \\ & \left\langle d_j^{(0)} \left| V \right| d_i^{(0)} \right\rangle = \Delta_{d_i}^{(1)} \delta_{ij} \end{aligned} \quad (9)$$

which solves for the first order energy drift $\Delta_{d_i}^{(1)}$, and at the same time shows the requirement that the restriction of V on D must be diagonalized by the basis $\left\{ \left| d_i^{(0)} \right\rangle \right\}$.

Let P_D be the projection operator onto subspace D , more explicitly

$$P_D = \sum_{i=1}^g \left| d_i^{(0)} \right\rangle \left\langle d_i^{(0)} \right| \quad (10)$$

and let $P_{\tilde{D}} = 1 - P_D$ be the projection operator onto D 's complement subspace \tilde{D} .

Our strategy for solving $\left| d_i^{(1)} \right\rangle$ is by solving for its components in D (i.e., $P_D \left| d_i^{(1)} \right\rangle$) and \tilde{D} (i.e., $P_{\tilde{D}} \left| d_i^{(1)} \right\rangle$) respectively. The reason is in \tilde{D} , $E_D^{(0)} - H_0$ is non-singular and hence invertible.

Rewrite (7) as

$$\begin{aligned} V \left| d_i^{(0)} \right\rangle &= (E_D^{(0)} - H_0) (P_D + P_{\tilde{D}}) \left| d_i^{(1)} \right\rangle + \Delta_{d_i}^{(1)} \left| d_i^{(0)} \right\rangle \\ &= \underbrace{(E_D^{(0)} - H_0) P_D \left| d_i^{(1)} \right\rangle}_{=0} + (E_D^{(0)} - H_0) P_{\tilde{D}} \left| d_i^{(1)} \right\rangle + \Delta_{d_i}^{(1)} \left| d_i^{(0)} \right\rangle \end{aligned} \quad (11)$$

Left-apply $P_{\tilde{D}}$ to (11), we get

$$\begin{aligned} P_{\tilde{D}} V \left| d_i^{(0)} \right\rangle &= P_{\tilde{D}} (E_D^{(0)} - H_0) P_{\tilde{D}} \left| d_i^{(1)} \right\rangle + \overbrace{P_{\tilde{D}} \Delta_{d_i}^{(1)} \left| d_i^{(0)} \right\rangle}^{=0} \\ &= (E_D^{(0)} - H_0) P_{\tilde{D}} \left| d_i^{(1)} \right\rangle \end{aligned} \quad (12)$$

where we have used $P_D H_0 = H_0 P_D$ (hence $P_{\tilde{D}} H_0 = H_0 P_{\tilde{D}}$).

Given (12), we can easily solve for $P_{\tilde{D}} \left| d_i^{(1)} \right\rangle$ by inverting non-singular operator $E_D^{(0)} - H_0$ defined over \tilde{D} ,

$$P_{\tilde{D}} \left| d_i^{(1)} \right\rangle = (E_D^{(0)} - H_0)^{-1} P_{\tilde{D}} V \left| d_i^{(0)} \right\rangle = \sum_{p^{(0)} \in \tilde{D}} \frac{\left| p^{(0)} \right\rangle \left\langle p^{(0)} \right| V \left| d_i^{(0)} \right\rangle}{E_D^{(0)} - E_p^{(0)}} \quad (13)$$

where the sum is over any set of 0th order eigenket of subspace \tilde{D} .

Now left-apply P_D to (8)

$$\begin{aligned} \overbrace{P_D (E_D^{(0)} - H_0) \left| d_i^{(2)} \right\rangle}^{=0} + P_D \Delta_{d_i}^{(1)} \left| d_i^{(1)} \right\rangle + P_D \Delta_{d_i}^{(2)} \left| d_i^{(0)} \right\rangle &= P_D V \left| d_i^{(1)} \right\rangle \\ \Delta_{d_i}^{(1)} P_D \left| d_i^{(1)} \right\rangle + \Delta_{d_i}^{(2)} \left| d_i^{(0)} \right\rangle &= P_D V P_D \left| d_i^{(1)} \right\rangle + P_D V P_{\tilde{D}} \left| d_i^{(1)} \right\rangle \end{aligned} \quad \Rightarrow \quad (14)$$

We can certainly write $P_D \left| d_i^{(1)} \right\rangle$ as a linear combination of D 's basis:

$$P_D \left| d_i^{(1)} \right\rangle = \sum_{k=1}^g a_{ik} \left| d_k^{(0)} \right\rangle \quad (15)$$

Plug (15) into (14) then left-apply $\left\langle d_j^{(0)} \right|$, we have

$$a_{ij} \Delta_{d_i}^{(1)} + \delta_{ij} \Delta_{d_i}^{(2)} = \sum_k a_{ik} \left\langle d_j^{(0)} \right| V \left| d_k^{(0)} \right\rangle + \left\langle d_j^{(0)} \right| V P_{\tilde{D}} \left| d_i^{(1)} \right\rangle \quad (16)$$

By (9), the first term on the RHS is $a_{ij} \Delta_{d_j}^{(1)}$. Furthermore, define

$$W \equiv \sum_{p^{(0)} \in \tilde{D}} \frac{V \left| p^{(0)} \right\rangle \left\langle p^{(0)} \right| V}{E_D^{(0)} - E_p^{(0)}} \quad (17)$$

(16) becomes

$$a_{ij} (\Delta_{d_i}^{(1)} - \Delta_{d_j}^{(1)}) + \delta_{ij} \Delta_{d_i}^{(2)} = \left\langle d_j^{(0)} \right| W \left| d_i^{(0)} \right\rangle \quad (18)$$

When $j = i$, a_{ij} vanishes by (3), which gives

$$\Delta_{d_i}^{(2)} = \left\langle d_i^{(0)} \right| W \left| d_i^{(0)} \right\rangle \quad (19)$$

For $j \neq i$, (18) becomes

$$a_{ij} (\Delta_{d_i}^{(1)} - \Delta_{d_j}^{(1)}) = \left\langle d_j^{(0)} \right| W \left| d_i^{(0)} \right\rangle \quad (20)$$

We have to consider two cases where

1. λ^1 perturbation has fully lifted the original degeneracy, i.e., $\Delta_{d_i}^{(1)} - \Delta_{d_j}^{(1)} \neq 0$ for $j \neq i$, and
2. λ^1 perturbation was not strong enough to lift the degeneracy in $\Delta_{d_i}^{(1)} = \Delta_{d_j}^{(1)}$.

In the case where degeneracy was lifted by λ^1 perturbation, we have

$$a_{ij} = \frac{\langle d_j^{(0)} | W | d_i^{(0)} \rangle}{\Delta_{d_i}^{(1)} - \Delta_{d_j}^{(1)}} \quad (21)$$

which, in combination of (15) and (13), gives the full 1st order eigenket $|d_i^{(1)}\rangle$.

In the second case, we can take all the $|d_i^{(0)}\rangle$ s that evaluate to the same value of $\nu = \Delta_{d_i}^{(1)} = \langle d_i^{(0)} | V | d_i^{(0)} \rangle$ and call the spanned subspace $F \subseteq D$. In this basis of F , the LHS of (20) vanishes when $i \neq j$, which means that W operator must be diagonal when restricted to F . Or equivalently, this requires that the choice of basis over F be the eigenkets of $W|_F$, i.e.,

$$\langle d_j^{(0)} | W|_F | d_i^{(0)} \rangle = \langle d_j^{(0)} | P_F W P_F | d_i^{(0)} \rangle = \delta_{ij} \Delta_{d_i}^{(2)} \quad (22)$$

To understand the whole picture qualitatively, when there is degeneracy in H_0 , we have freedom to choose any orthonormal 0th order basis over D . But if we consider 1st order theory, we require (9) which imposes restrictions upon our choice of basis over the degenerate subspace D . If this restriction is not enough to lift all the degeneracy, we may still have some remaining freedom to choose our basis in a smaller-but-more-degenerate subspace F , for which the 2nd order theory imposes more restrictions by requiring $W|_F$'s diagonality (22).

Now to solve for $P_D |d_i^{(1)}\rangle$ for $|d_i^{(0)}\rangle \in F$, we recurse our strategy earlier by trying to solve separately for $P_F |d_i^{(1)}\rangle$ and $P_{D \setminus F} |d_i^{(1)}\rangle$. For clarity, we now rename $|d_i\rangle$ as $|f_i\rangle$ to emphasize that we are now dealing with eigenkets whose 0th order are in $F \subseteq D$.

Recall that the membership in F (hence the degeneracy) prevents us from obtaining a_{ik} s in (15) by directly inverting $\Delta_{f_i}^{(1)} - \Delta_{f_j}^{(1)}$ in (18). So let's rewrite $\Delta_{f_i}^{(1)}$ as $\Delta_F^{(1)}$ to highlight the common degenerate value over F , and break up $P_D |f_i^{(1)}\rangle$ into $(P_D + P_{D \setminus F}) |f_i^{(1)}\rangle$ in (14):

$$\begin{aligned} (\Delta_F^{(1)} - P_D V) P_F |f_i^{(1)}\rangle + (\Delta_F^{(1)} - P_D V) P_{D \setminus F} |f_i^{(1)}\rangle + \Delta_{f_i}^{(2)} |f_i^{(0)}\rangle &= P_D V P_D |f_i^{(1)}\rangle \\ \text{by (13), (17)} &= P_D W |f_i^{(0)}\rangle \end{aligned} \quad (23)$$

Left-apply $P_{D \setminus F}$ to (23):

$$P_{D \setminus F} (\Delta_F^{(1)} - P_D V) P_F |f_i^{(1)}\rangle + P_{D \setminus F} (\Delta_F^{(1)} - P_D V) P_{D \setminus F} |f_i^{(1)}\rangle + P_{D \setminus F} \Delta_{f_i}^{(2)} |f_i^{(0)}\rangle = P_{D \setminus F} P_D W |f_i^{(0)}\rangle \quad (24)$$

Now the first term on the LHS of (24) vanishes because $P_{D \setminus F} P_F = 0$, as well as $P_{D \setminus F} P_D V P_F = P_{D \setminus F} V P_F = 0$ by diagonality of V over D . The third term also drops out since $P_{D \setminus F} |f_i^{(0)}\rangle$ vanishes. What's remaining of (24) becomes

$$(\Delta_F^{(1)} - P_{D \setminus F} V P_{D \setminus F}) P_{D \setminus F} |f_i^{(1)}\rangle = P_{D \setminus F} W |f_i^{(0)}\rangle \quad (25)$$

for which we can easily solve for $P_{D \setminus F} |f_i^{(1)}\rangle$ by inverting the non-singular operator $\Delta_F^{(1)} - P_{D \setminus F} V P_{D \setminus F}$ over the domain $D \setminus F$, i.e.,

$$P_{D \setminus F} |f_i^{(1)}\rangle = (\Delta_F^{(1)} - P_{D \setminus F} V P_{D \setminus F})^{-1} P_{D \setminus F} W |f_i^{(0)}\rangle = \sum_{q^{(0)} \in D \setminus F} \frac{|q^{(0)}\rangle \langle q^{(0)} | W | f_i^{(0)} \rangle}{\Delta_F^{(1)} - \Delta_q^{(1)}} \quad (26)$$

where the sum is over the set of 0th order eigenket of subspace $D \setminus F$.

One can't help noticing the structural similarity between (13) and (26), with $D \setminus F$ replacing \tilde{D} and W replacing V , etc.

We will go one step further to make the pattern more manifest. Assuming the existence of F -degeneracy, now we try to find the remaining components $P_F |f_i^{(1)}\rangle$.

Notice that we haven't left-applied $P_{\tilde{D}}$ to (8) yet, let's do just that:

$$\begin{aligned} P_{\tilde{D}}(E_D^{(0)} - H_0) \left| f_i^{(2)} \right\rangle + P_{\tilde{D}} \Delta_{f_i}^{(1)} \left| f_i^{(1)} \right\rangle + \overbrace{P_{\tilde{D}} \Delta_{f_i}^{(2)} \left| f_i^{(0)} \right\rangle}^{=0} &= P_{\tilde{D}} V \left| f_i^{(1)} \right\rangle \\ (E_D^{(0)} - H_0) P_{\tilde{D}} \left| f_i^{(2)} \right\rangle &= -\Delta_F^{(1)} P_{\tilde{D}} \left| f_i^{(1)} \right\rangle + P_{\tilde{D}} V (P_{\tilde{D}} + P_{D \setminus F} + P_F) \left| f_i^{(1)} \right\rangle \end{aligned} \quad \Rightarrow \quad (27)$$

Invert non-singular operator $E_D^{(0)} - H_0$ over domain \tilde{D} ,

$$\begin{aligned} P_{\tilde{D}} \left| f_i^{(2)} \right\rangle &= (E_D^{(0)} - H_0)^{-1} \left[-\Delta_F^{(1)} P_{\tilde{D}} \left| f_i^{(1)} \right\rangle + P_{\tilde{D}} V P_{\tilde{D}} \left| f_i^{(1)} \right\rangle + P_{\tilde{D}} V P_{D \setminus F} \left| f_i^{(1)} \right\rangle \right] + (E_D^{(0)} - H_0)^{-1} P_{\tilde{D}} V P_F \left| f_i^{(1)} \right\rangle \\ &= A \left| f_i^{(0)} \right\rangle + (E_D^{(0)} - H_0)^{-1} P_{\tilde{D}} V P_F \left| f_i^{(1)} \right\rangle \end{aligned} \quad (28)$$

where we have used (13) and (26) to convert the square bracket as a linear combination of $\left| f_i^{(0)} \right\rangle$ that is represented by the overall operator A .

Continuing (6)-(8), we have the λ^3 order equation

$$\lambda^3 \text{ order :} \quad (E_D^{(0)} - H_0) \left| f_i^{(3)} \right\rangle + \Delta_{f_i}^{(1)} \left| f_i^{(2)} \right\rangle + \Delta_{f_i}^{(2)} \left| f_i^{(1)} \right\rangle + \Delta_{f_i}^{(3)} \left| f_i^{(0)} \right\rangle = V \left| f_i^{(2)} \right\rangle \quad (29)$$

Left-apply P_F to (29), notice the first term will vanish by virtue of $F \subseteq D$, we obtain:

$$\begin{aligned} \Delta_{f_i}^{(1)} P_F \left| f_i^{(2)} \right\rangle + \Delta_{f_i}^{(2)} P_F \left| f_i^{(1)} \right\rangle + \Delta_{f_i}^{(3)} \left| f_i^{(0)} \right\rangle &= P_F V \left| f_i^{(2)} \right\rangle \\ &= P_F V (P_{\tilde{D}} + P_{D \setminus F} + P_F) \left| f_i^{(2)} \right\rangle \\ &= P_F V P_{\tilde{D}} \left| f_i^{(2)} \right\rangle + \overbrace{P_F V P_{D \setminus F} \left| f_i^{(2)} \right\rangle}^{=0} + P_F V P_F \left| f_i^{(2)} \right\rangle \end{aligned} \quad (30)$$

where the second term on the RHS vanishes because $V|_D$ is diagonal.

Rearrange the terms and notice that $\Delta_{f_i}^{(1)} P_F - P_F V P_F = (\Delta_F^{(1)} - P_F V P_F) P_F = 0$ because $\Delta_F^{(1)}$ is the common degenerate eigenvalue of V restricted to F . Then (30) becomes

$$\begin{aligned} \Delta_{f_i}^{(2)} P_F \left| f_i^{(1)} \right\rangle + \Delta_{f_i}^{(3)} \left| f_i^{(0)} \right\rangle &= P_F V P_{\tilde{D}} \left| f_i^{(2)} \right\rangle \quad \text{by (28)} \Rightarrow \\ \left[\Delta_{f_i}^{(2)} - P_F \underbrace{V (E_D^{(0)} - H_0)^{-1} P_{\tilde{D}} V P_F}_{=W} \right] P_F \left| f_i^{(1)} \right\rangle + \Delta_{f_i}^{(3)} \left| f_i^{(0)} \right\rangle &= P_F V A \left| f_i^{(0)} \right\rangle \quad \Rightarrow \\ (\Delta_{f_i}^{(2)} - P_F W P_F) P_F \left| f_i^{(1)} \right\rangle + \Delta_{f_i}^{(3)} \left| f_i^{(0)} \right\rangle &= P_F V A \left| f_i^{(0)} \right\rangle \end{aligned} \quad (31)$$

Now (31) is exactly the recurrence of the situation in (14)-(18). We immediately know that if we write

$$P_F \left| f_i^{(1)} \right\rangle = \sum_k b_{ik} \left| f_k^{(0)} \right\rangle \quad (32)$$

we will get the recurrence of (18)

$$b_{ij} (\Delta_{f_i}^{(2)} - \Delta_{f_j}^{(2)}) + \delta_{ij} \Delta_{f_i}^{(3)} = \left\langle f_j^{(0)} \right| V A \left| f_i^{(0)} \right\rangle \quad (33)$$

If the 2nd-order degeneracy is lifted, i.e., $\Delta_{f_i}^{(2)} \neq \Delta_{f_j}^{(2)}$ when $i \neq j$, we can solve directly for $P_F \left| f_i^{(1)} \right\rangle$ (thus completing the calculation for $\left| f_i^{(1)} \right\rangle$ by combining its $D \setminus F$ and \tilde{D} components obtained earlier). Otherwise, the remaining 2nd-order degeneracy dictates the 3rd-order restriction that the basis of the now even-smaller degenerate subspace $G \subseteq F$ must diagonalize VA . Obviously we can continue this fashion to the higher order.

Finally, let's summarize the strategy to solve degenerate perturbation to arbitrary orders:

1. We start with a degenerate subspace D whose set of basis $\left| d_i^{(0)} \right\rangle$ all satisfy the 0th order eigenequation. At 0th order, due to the degeneracy, we have freedom to choose any orthonormal linear combination of them as a valid basis.
2. For λ^1 perturbation theory, another operator V was introduced to the scene. The 0th order degeneracy in D restricts the choice $\left| d_i^{(0)} \right\rangle$ to be the eigenkets of V (eq (9)), which reduces the freedom of choice for D 's basis.

3. The 1st order energy shift $\Delta_{d_i}^{(1)}$ corresponds to the diagonal element of V in this basis (eq (9)).
4. We can obtain the components of $P_{\tilde{D}} \left| d_i^{(1)} \right\rangle$ for the "out" subspace \tilde{D} regardless of whether $V|_D$ has degenerate diagonal element (eq (13)).
5. If V is not degenerate, we can directly obtain the "in" components $P_D \left| d_i^{(1)} \right\rangle$ (eq (21)) and we are back to the non-degenerate perturbation theory.
6. If V has degeneracy in a (potentially smaller) subspace $F \subseteq D$, let $\left| f_i^{(0)} \right\rangle$ be its basis, which at λ^1 order, has freedom of choice.
 - (a) Now we go to the λ^2 theory, which introduces a new operator W into the scene. At this order, the degeneracy of V in F requires $\left| f_i^{(0)} \right\rangle$ s to diagonalize W (eq (22)), which limits its freedom of choice.
 - (b) The 2nd order energy shift $\Delta_{f_i}^{(2)}$ corresponds to the diagonal element of W in this basis (eq (22)).
 - (c) We can obtain the components of $P_{D \setminus F} \left| f_i^{(1)} \right\rangle$ for the "out" subspace $D \setminus F$ regardless of whether $W|_F$ has degenerate diagonal element (eq (26)).
 - (d) If W is not degenerate, we can directly obtain the "in" components $P_F \left| f_i^{(1)} \right\rangle$ and we are back to the non-degenerate perturbation theory (eq (33)).
 - (e) If W has degeneracy in a (potentially smaller) subspace $G \subseteq F \subseteq D$, let $\left| g_i^{(0)} \right\rangle$ be its basis, which at λ^2 order, has freedom of choice.
 - i. Now we go to the λ^3 theory, which introduces a new operator VA into the scene. At this order, the degeneracy of W in G requires $\left| g_i^{(0)} \right\rangle$ s to diagonalize VA (eq (33)), which limits its freedom of choice.
 - ii. The 3rd order energy shift $\Delta_{g_i}^{(3)}$ corresponds to the diagonal element of VA in this basis (eq (33)).
 - iii. \dots
 - \dots