(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

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

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

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 $|d_i\rangle$ 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.,

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

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

The perturbed energy eigenequation is

$$(E_{d_i} - H_0)\,|d_i\rangle = \lambda V\,|d_i\rangle \tag{4}$$

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

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

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

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

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

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

(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

$$\underbrace{\left\langle d_j^{(0)}\middle|E_D^{(0)} - H_0\right.}_{=0}\left|d_i^{(1)}\right\rangle + \left\langle d_j^{(0)}\middle|\Delta_{d_i}^{(1)}\middle|d_i^{(0)}\right\rangle = \left\langle d_j^{(0)}\middle|V\middle|d_i^{(0)}\right\rangle \quad \Longrightarrow$$

$$\left\langle d_j^{(0)}\middle|V\middle|d_i^{(0)}\right\rangle = \Delta_{d_i}^{(1)}\delta_{ij} \tag{9}$$

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

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

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

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 $\widetilde{D}$ (i.e., $P_{\widetilde{D}}\left|d_i^{(1)}\right\rangle$) respectively. The reason is in $\widetilde{D}$, $E_D^{(0)}-H_0$ is non-singular and hence invertible.

Rewirte (7) as

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

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

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

where we have used $P_DH_0 = H_0P_D$ (hence $P_{\widetilde{D}}H_0 = H_0P_{\widetilde{D}}$).

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

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

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

Now left-apply P_D to (8)

$$\begin{aligned} \overbrace{P_D\left(E_D^{(0)}-H_0\right)}^{=0}\left|d_i^{(2)}\right\rangle + P_D\Delta_{d_i}^{(1)}\left|d_i^{(1)}\right\rangle + P_D\Delta_{d_i}^{(2)}\left|d_i^{(0)}\right\rangle = P_DV\left|d_i^{(1)}\right\rangle \qquad \Longrightarrow \\ \Delta_{d_i}^{(1)}P_D\left|d_i^{(1)}\right\rangle + \Delta_{d_i}^{(2)}\left|d_i^{(0)}\right\rangle = P_DVP_D\left|d_i^{(1)}\right\rangle + P_DVP_{\widetilde{D}}\left|d_i^{(1)}\right\rangle \end{aligned} \tag{14}$$

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

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

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

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

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

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

(16) becomes

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

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

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

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

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

We have to consider two cases where

1. λ^1 perturbation has fully lifted the original degeneracy, i.e., $\Delta^{(1)}_{d_i} - \Delta^{(1)}_{d_j} \neq 0$ for $j \neq i$, and

2. λ^1 perturbation was not strong enough to lift the degeneracy in $\Delta^{(1)}_{d_i} = \Delta^{(1)}_{d_j}$.

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

$$a_{ij} = \frac{\left\langle d_j^{(0)} \middle| W \middle| d_i^{(0)} \right\rangle}{\Delta^{(1)}_{d_i} - \Delta^{(1)}_{d_j}} \tag{21}$$

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

In the second case, we can take all the $\left| d_i^{(0)} \right\rangle$s that evaluate to the same value of $v = \Delta^{(1)}_{d_i} = \left\langle d_i^{(0)} \middle| V \middle| d_i^{(0)} \right\rangle$ 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.,

$$\left\langle d_j^{(0)} \middle| W|_F \middle| d_i^{(0)} \right\rangle = \left\langle d_j^{(0)} \middle| P_F W P_F \middle| d_i^{(0)} \right\rangle = \delta_{ij} \Delta^{(2)}_{d_i} \tag{22}$$

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. Buf 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 $P_D \left| d_i^{(1)} \right\rangle$ for $\left| d_i^{(0)} \right\rangle \in F$, we recurse our strategy earlier by trying to solve separately for $P_F \left| d_i^{(1)} \right\rangle$ and $P_{D \setminus F} \left| d_i^{(1)} \right\rangle$. 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 $\Delta^{(1)}_{f_i} - \Delta^{(1)}_{f_j}$ in (18). So let's rewrite $\Delta^{(1)}_{f_i}$ as $\Delta^{(1)}_F$ to highlight the common degenerate value over F, and break up $P_D \left| f_i^{(1)} \right\rangle$ into $\left(P_D + P_{D \setminus F}\right) \left| f_i^{(1)} \right\rangle$ in (14):

$$\begin{aligned} \left(\Delta^{(1)}_F - P_D V\right) P_F \left| f_i^{(1)} \right\rangle + \left(\Delta^{(1)}_F - P_D V\right) P_{D \setminus F} \left| f_i^{(1)} \right\rangle + \Delta^{(2)}_{f_i} \left| f_i^{(0)} \right\rangle &= P_D V P_{\widetilde{D}} \left| f_i^{(1)} \right\rangle \\ \text{by (13), (17)} \qquad &= P_D W \left| f_i^{(0)} \right\rangle \end{aligned} \tag{23}$$

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

$$P_{D \setminus F} \left(\Delta^{(1)}_F - P_D V\right) P_F \left| f_i^{(1)} \right\rangle + P_{D \setminus F} \left(\Delta^{(1)}_F - P_D V\right) P_{D \setminus F} \left| f_i^{(1)} \right\rangle + P_{D \setminus F} \Delta^{(2)}_{f_i} \left| f_i^{(0)} \right\rangle = P_{D \setminus F} P_D W \left| f_i^{(0)} \right\rangle \tag{24}$$

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 $P_{D \setminus F} \left| f_i^{(0)} \right\rangle$ vanishes. What's remaining of (24) becomes

$$\left(\Delta^{(1)}_F - P_{D \setminus F} V P_{D \setminus F}\right) P_{D \setminus F} \left| f_i^{(1)} \right\rangle = P_{D \setminus F} W \left| f_i^{(0)} \right\rangle \tag{25}$$

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

$$P_{D \setminus F} \left| f_i^{(1)} \right\rangle = \left(\Delta^{(1)}_F - P_{D \setminus F} V P_{D \setminus F}\right)^{-1} P_{D \setminus F} W \left| f_i^{(0)} \right\rangle = \sum_{q^{(0)} \in D \setminus F} \frac{\left| q^{(0)} \right\rangle \left\langle q^{(0)} \middle| W \middle| f_i^{(0)} \right\rangle}{\Delta^{(1)}_F - \Delta^{(1)}_q} \tag{26}$$

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 $\widetilde{D}$ 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 $P_F \left| f_i^{(1)} \right\rangle$.

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

$$P_{\widetilde{D}}\left(E_D^{(0)}-H_0\right)\left|f_i^{(2)}\right\rangle+P_{\widetilde{D}}\Delta_{f_i}^{(1)}\left|f_i^{(1)}\right\rangle+\overbrace{P_{\widetilde{D}}\Delta_{f_i}^{(2)}\left|f_i^{(0)}\right\rangle}^{=0}=P_{\widetilde{D}}V\left|f_i^{(1)}\right\rangle \qquad \Longrightarrow$$
$$\left(E_D^{(0)}-H_0\right)P_{\widetilde{D}}\left|f_i^{(2)}\right\rangle=-\Delta_F^{(1)}P_{\widetilde{D}}\left|f_i^{(1)}\right\rangle+P_{\widetilde{D}}V\left(P_{\widetilde{D}}+P_{D\setminus F}+P_F\right)\left|f_i^{(1)}\right\rangle \tag{27}$$

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

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

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

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

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

$$\begin{aligned}\Delta_{f_i}^{(1)}P_F\left|f_i^{(2)}\right\rangle+\Delta_{f_i}^{(2)}P_F\left|f_i^{(1)}\right\rangle+\Delta_{f_i}^{(3)}\left|f_i^{(0)}\right\rangle&=P_FV\left|f_i^{(2)}\right\rangle\\&=P_FV\left(P_{\widetilde{D}}+P_{D\setminus F}+P_F\right)\left|f_i^{(2)}\right\rangle\\&=P_FVP_{\widetilde{D}}\left|f_i^{(2)}\right\rangle+\overbrace{P_FVP_{D\setminus F}}^{=0}\left|f_i^{(2)}\right\rangle+P_FVP_F\left|f_i^{(2)}\right\rangle\end{aligned} \tag{30}$$

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

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

$$\begin{aligned}\Delta_{f_i}^{(2)}P_F\left|f_i^{(1)}\right\rangle+\Delta_{f_i}^{(3)}\left|f_i^{(0)}\right\rangle&=P_FVP_{\widetilde{D}}\left|f_i^{(2)}\right\rangle \qquad \text{by (28)} \Longrightarrow\\ \left[\Delta_{f_i}^{(2)}-P_F\underbrace{V\left(E_D^{(0)}-H_0\right)^{-1}P_{\widetilde{D}}V}_{=W}P_F\right]P_F\left|f_i^{(1)}\right\rangle+\Delta_{f_i}^{(3)}\left|f_i^{(0)}\right\rangle&=P_FVA\left|f_i^{(0)}\right\rangle \qquad \Longrightarrow\\ \left(\Delta_{f_i}^{(2)}-P_FWP_F\right)P_F\left|f_i^{(1)}\right\rangle+\Delta_{f_i}^{(3)}\left|f_i^{(0)}\right\rangle&=P_FVA\left|f_i^{(0)}\right\rangle\end{aligned} \tag{31}$$

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

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

we will get the recurrence of (18)

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

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 $\widetilde{D}$ 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 $P_{\widetilde{D}} \left| d_i^{(1)} \right\rangle$ for the "out" subspace $\widetilde{D}$ 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. $\cdots$

      $\cdots$