Messiah Chapter 16 Stationary Perturbation Theory Notes, Round Two PhL 1.23.09

symbol grab: $\Sigma_{k\in\mathcal{L}_\perp}\ \mathcal{H}^{(m)}\oplus\mathcal{H}^{\perp}\ \mathcal{E}_a{}^0\ (\mathcal{E}_a{}^0)^{\perp}\in\subset$

I am not ready for "meta notes" yet. Here we take a second pass through Messiah's offering, and I try to impose my own structure on his information, adding details where I think useful.

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Topic I. The Non-Degenerate Case (686)

Actually, I am going to try to stay as general as possible (ie, allow degeneracy) except where stated otherwise.

2. Expansion in Powers of the Perturbation (686)

3. First Order Perturbations (688)
6. Higher Order Corrections (694)

Everything done here is analogous to Schiff (which I read first), but the notation is different, so here is a summary of the notation comparison:

Schiff/PL	Messiah	
m	a	// selected state (or space of N degenerate states)
$\mathcal{H}^{0(m)}$	$\mathcal{E}_a{}^0$	// space containing N deg unperturbed state(s) of interest
$\mathcal{H}^{(m)}$	$\mathcal{E}_a$	// space containing the N perturbed states
$\mathcal{H} = \mathcal{H}^0$	$\mathcal{H} = \mathcal{H}^0$	// full Hilbert space
H'	V	// perturbing Hamiltonian
$W_m = \Sigma_{n=0}\, \lambda^n\, W_{m,n}$	$E = E_a{}^0 + \Sigma_{n=1}\, \lambda^n\, \varepsilon_n$	// energy expansion
W_m	E_a	
$W_{m,0}$	$E_a{}^0$	
$W_{m,n}$	ε_n	n = 1,2,3...
$\psi_m = \Sigma_{n=0}\, \lambda^n\, \psi_{m,n}$	$\lvert\psi\rangle = \Sigma_{n=0}\, \lambda^n\, \lvert n\rangle$	// state expansion
$\psi_{m,n}$	$\lvert n\rangle$ n = 0,1,2....	// the tag "a" is implicit
$\langle u_m \lvert \psi_{m,n}\rangle = 0$ n>0	$\langle 0 \lvert n\rangle = 0$ n>0	// special normalization

The Main Equation set for perturbation theory is 31.4 in Schiff and appears as (7) page 687 in Messiah. Before we get to it, there are many "preliminaries" to be considered. There are several totally new ingredients in Messiah not present in Schiff.

a. Mapping Notations → and ⇒, and the Inverse of a Linear Operator

Consider an operator Ω_0: $\mathcal{H}^0 \rightarrow \mathcal{H}^0$. For bound state problems, $\mathcal{H}^0$ could be either a finite or infinite dimensional Hilbert Space (we sort of ignore the continuous part of the spectrum, the collision part for H). When we "mess with operators", we are *in general* trying to find equations that are valid in all of $\mathcal{H}^0$ so we can use them freely. In the above notation, $\mathcal{H}^0 \rightarrow \mathcal{H}^0$ shows the two *spaces* involved, it does not show what the domain and range actually might be for Ω_0 , and you really need to know these two things about Ω_0 to use it. Usually in our application the domain will be all of $\mathcal{H}^0$. We know that if Ω_0 has a non-trivial nullspace and if it is Hermitian or symmetric or self-adjoint of whatever, then the Alternative Theorem tells us that the range is less than all of $\mathcal{H}^0$. More simply put, if $Ax_0 = 0$, then the problem Ax=f which has a solution (x,f) also has a solution $A(x+x_0) = f$ so that the image vector f maps back into lots of domain vectors, which means A is not one-to-one and this means A^{-1} *does not exist*. This fact is true regardless of the dimension of $\mathcal{H}^0$, finite or infinite. If we know that Ω_0 has a certain range when the domain is all of $\mathcal{H}^0$, we will use this notation to show that fact: Ω_0: $\mathcal{H}^0 \Rightarrow \mathcal{R}^0$. This is my own made-up notation just to clarify this precise point, Ω_0:domain ⇒ range. The various 0's here just remind us we are talking about the unperturbed state Hilbert Space $\mathcal{H}^0$.

b. The General Projection operator R

Suppose also that R is a projection operator R: $\mathcal{H}^0 \Rightarrow$ S which projects onto some subspace S in $\mathcal{H}$. Then as above, we have R representable as "a portion of unity":

$$R = \Sigma_{r \in S} |r><r| \qquad 1 = \Sigma_{n,all} |n><n|$$

where in general |k> form an orthonormal basis for $\mathcal{H}^0$. It is easy to show that $R^2 = R$: just put in the sums shown and use $<r|r'> = \delta_{r,r'}$. It is also easy to show that $R = R^\dagger$. The simplest proof is to realize that $[|r>]^\dagger = <r|$ and similarly for the ket. Perhaps a more convincing proof is this:

$$R_{ij} = <i|R|j> = \Sigma_{r \in S} <i \mid r><r \mid j> = \Sigma_{r \in S} <r \mid j><i \mid r> = \Sigma_{r \in S} <j \mid r>^*<r \mid i>^* = R_{ji}^* = (R^\dagger)_{ij}$$

where i and j can be any states, not just basis states. If we use basis states, then we have

$$R_{ij} = <i|R|j> = \Sigma_{r \in S} <i \mid r><r \mid j> = \delta_{i,j} \text{ if both in S, else = 0}$$

and then we see that R_{ij} is just a partially populated unit matrix (a portion of unity) which of course is Hermitian, and Hermiticity is in invariant under any unitary transformation to another basis, so R is Hermitian in any basis. So, our main ideas here are these:

$$R: \mathcal{H}^0 \rightarrow \mathcal{H}^0 \qquad R: \mathcal{H}^0 \Rightarrow S \qquad R^2 = R \qquad R = R^\dagger$$

$$R|r> = |r>, r \in S \qquad R|k> = 0, \; k \in S^\perp \qquad R^{-1} \text{ does not exist}$$

where the last follows since R has a non-trivial nullspace $S^\perp$ as shown on the same line.

c. Projection operators P_0 and Q_0

The first *new ingredient*s appearing in Messiah are the P_0 and Q_0 operators. P_0: $\mathcal{H}^0 \Rightarrow \mathcal{E}_a{}^0$ is very clear as a projection operator. It's partner is Q_0: $\mathcal{H}^0 \Rightarrow (\mathcal{E}_a{}^0)^\perp$ and of course $P_0 + Q_0 = 1$. Really these things should be called P_{a0} and Q_{a0}. Later on, he introduces an analogous operator P: $\mathcal{H} \rightarrow \mathcal{E}_a$, but we won't need that for a while. Here are some good equations:

$P_0 = \Sigma_{j \in \mathcal{E}_{0a}} |j><j|$ // portion of full unity accounted for by the $\mathcal{E}_a{}^0$ subspace

$Q_0 = \Sigma_{k \in \mathcal{E}_{0a}\perp} |k><k|$ // portion of full unity accounted for by all other states in $\mathcal{H}^0$

$1 = \Sigma_n |n><n|$ // sum over all states gives the full unity

$P_0Q_0 = Q_0P_0 = 0$ // should be obvious

$P_0^2 = P_0$ and $P_0^\dagger = P_0$ and $Q_0^2 = Q_0$ and $Q_0^\dagger = Q_0$

Warning: We know that $P_0^2 = 1$. If we write $1 = P_0 P_0^{-1}$ then we are tempted to say that $P_0^{-1} = P_0$. This is wrong! Because the range of P_0 is less than $\mathcal{H}^0$ (or because P_0 has a non-trivial nullspace), we know (as just discussed above) that the operator P_0^{-1} *does not exist*, so don't try to use it in any calculations! This applies to any projection operator, and hence to Q_0 as well.

d. Projection-Sandwich Operators in $\mathcal{H}$

Suppose Ω is diagonal in our selected basis for space $\mathcal{H}$ with eigenvalues ω_k. Suppose also that R is a projection operator which projects onto some subspace S in $\mathcal{H}$. Then as above, we have

$$R = \Sigma_{r \in S} |r><r|$$

Consider then this combination operator

$$F = R\, f(\Omega)\, R \qquad (1)$$

where we sandwich an arbitrary function of Ω between two copies of our projection operator. It is trivial then to show that (the eigenvalues ω_r need not be real)

$$F = \Sigma_{r \in S} |r>\, f(\omega_r) <r| \qquad (2)$$

Here we use the tradition of putting the *number* $f(\omega_r)$ in the middle, but it could go anywhere:

$$\Sigma_{r \in S} |r> C_r <r| \;= \Sigma_{r \in S} C_r\, |r> <r| \;= \Sigma_{r \in S}\, |r> <r|\, C_r$$

because this thing is just a linear combination of operators $|r> <r|$ with coefficient C_r.

As a special case, suppose $f(\Omega) = \Omega^{-1}$ (which we assume exists). Then we have

$$F = R\, \Omega^{-1}\, R \;=\; \Sigma_{r \in S} |r>\, (1/\omega_r) <r| \qquad (3)$$

where we assume $\omega_r \neq 0$ at least in the set S. Then we find this interesting result:

$$\Omega\, F \;= R \qquad (4)$$

Just insert the expansion and use $\Omega\ |r> = \omega_r\ |r>$ and then you get $(1/\omega_r)\omega_r = 1$ and you end up with R. The above implies that $F^\dagger\, \Omega^\dagger \;= R$. If Ω is Hermitian, then so is F and we have

$$F\, \Omega \;= R \qquad // \ \Omega = \Omega^\dagger \qquad (5)$$

In this case, we also have that

$$F\, \Omega |r_1> = R|r_1> = |r_1> \qquad // \ \Omega = \Omega^\dagger \qquad (6)$$

This says that for such a state, F acts in effect as the inverse of Ω, nothing very profound.

Now here is another theorem that is easy to prove

$$F_1F_2F_3 = R\, f_1(\Omega)\, R\, R\, f_2(\Omega)\, R\, R\, f_3(\Omega)\, R = R\, f_1(\Omega)\, R f_2(\Omega)\, R f_3(\Omega)\, R \qquad (7)$$
$$= \Sigma_{r\in S} |r\rangle\, f_1(\omega_r)\, f_2(\omega_r)\, f_3(\omega_r)\langle r|$$

In this proof, we took every $f_i(\Omega)$ and acted to the right on $|r\rangle$ to get $f_i(\omega_r)\,|r\rangle$ and then we used $\langle r|r'\rangle = \delta_{r,r'}$ on three of the r sums. You can never get rid of the last sum! This result does not require f_i to be a real function nor does it require that the ω_r be real. As a special case of the above theorem we have the leftmost equality here

$$F^n = \Sigma_{r\in S} |r\rangle\, f(\omega_r)^n \langle r| = R\, f(\Omega)^n\, R \qquad (8)$$

and the rightmost equality follows trivially by -- as usual -- inserting the expansion for R.

e. The operator Q_{0a}

This operator is a special case of the above where $R = Q_0$ and $\Omega = (E_a^0\, 1 - H_0) = (E_a^0 - H_0)$. Recall that Q_0 projects onto the perp space of our space $\mathcal{E}_a^0$ "of interest". So

$$Q_{0a} \equiv Q_0\, (E_a^0 - H_0)^{-1} Q_0 = -\, Q_0\, G_0\, Q_0$$

where both Q_0 and H_0 on the RHS are operators, and of course E_a^0 is just a number. Later we might refer to this central operator $(E_a^0 - H_0)^{-1}$ as (minus) the unperturbed resolvent G_0, and I show that on the right above. Quoting result (d.8) above we have

$$(Q_{0a})^n = Q_0\, (E_a^0 - H_0)^{-n} Q_0 = \Sigma_{k\in\mathcal{E}_{0a}\perp} |k\rangle\, (E_a^0 - E_k^0)^{-n}\, \langle k| = "\ \frac{Q_0}{a^n}\ "$$

Because the operator $(Q_{0a})^n$ has Q_0 on each end, it becomes 0 if it is pressed against a P_0 operator on either the left or right. For example, consider this where we have lots of operators:

$$ABC....FP_0(Q_{0a})^nXY...Z = ABC....F\,(Q_{0a})^n\, P_0XY...Z = 0$$

Messiah uses the exceedingly unhelpful notation shown on the right to represent $(Q_{0a})^n$. It is meant to remind the user that $(E_a^0 - E_k^0)^{-n}$ symbolized by a^{-n} is sandwiched between the normal Q_0 operators. I don't use this notation in any of my notes.

Notice that $\Omega = (E_a^0 - H_0)$ is Hermitian, so as noted above before (5), Q_{0a} is also Hermitian, so we get both results (4) and (5) ,

$$\Omega F = R = F\Omega \qquad F = R\ \Omega^{-1}\ R$$

$$(E_a^0 - H_0)\, Q_{0a} = Q_0 = Q_{0a}\, (E_a^0 - H_0) \qquad Q_{0a} \equiv Q_0\, (E_a^0 - H_0)^{-1} Q_0$$

f. Does $\Omega^{-1} = (E_a^0 - H_0)^{-1}$ exist?

The SE tells us that $H_o|\psi> = E_a^0|\psi>$ for any ψ inside $\mathcal{E}_a^0$. Thus, we know that $(E_a^0 - H_0)\ |\psi>= 0$ so the operator $(E_a^0 - H_0)$ clearly has some non-trivial nullspace. We therefore know that $(E_a^0 - H_0)^{-1}$ *does not* exist if we think of $(E_a^0 - H_0)$: $\mathcal{H}^0 \rightarrow \mathcal{H}^0$.

However, we can also think of a different operator $(E_a^0 - H_0)$: $(\mathcal{E}_a^0)^\perp \rightarrow (\mathcal{E}_a^0)^\perp$ where we have changed the mapping spaces. This is not domain and range necessarily, we use the $\rightarrow$ notation to refer to the spaces. Each space here is in fact a Hilbert Space, by the way. For any state $|k>$ in $(\mathcal{E}_a^0)^\perp$, we know that the SE says $H_o|k> = E_k^0|k>$ where $E_k^0 \neq E_a^0$. So yes, $(E_k^0 - H_0)\ |k> = 0$. But then we have

$$(E_a^0 - H_0)\ |k> = (E_a^0 - H_0 + E_k^0 - E_k^0)\ |k> = (E_a^0 - E_k^0)\ |k> \neq 0 \qquad |k> \in (\mathcal{E}_a^0)^\perp$$

Since we get $\neq 0$ for all basis kets in $(\mathcal{E}_a^0)^\perp$, it is clear that we get $\neq 0$ for any ket in $(\mathcal{E}_a^0)^\perp$. Since we never get 0, that means $(E_a^0 - H_0)$ has only the trivial nullspace in $(\mathcal{E}_a^0)^\perp$ and thus $(E_a^0 - H_0)^{-1}$ exists, where we have now carefully restricted what we mean by $(E_a^0 - H_0)$.

Now consider again $Q_{0a} \equiv Q_0\ (E_a^0 - H_0)^{-1} Q_0$. The central part here $(E_a^0 - H_0)^{-1}$ can never act on a ket in $\mathcal{E}_a^0$! It has "protectors" on each side, in the form of Q_0. Thus, in effect, $(E_a^0 - H_0)^{-1}$ here can only act on $|k>$ or $<k| \in (\mathcal{E}_a^0)^\perp$! This is I think a key fact about this Q_{0a} operator! You can think of this really as the product of three operator acting left to right as follows (we start on with the left Q_0)

$$Q_0 : \mathcal{H}^0 \Rightarrow (\mathcal{E}_a^0)^\perp \quad (E_a^0 - H_0)^{-1} : (\mathcal{E}_a^0)^\perp \rightarrow (\mathcal{E}_a^0)^\perp \quad Q_0 : (\mathcal{E}_a^0)^\perp \Rightarrow (\mathcal{E}_a^0)^\perp$$

$$Q_{0a} : \mathcal{H}^0 \Rightarrow (\mathcal{E}_a^0)^\perp \quad \text{overall}$$

The last Q_0 does not do anything when viewed this way, but we can alternatively think of the three operators as acting in the reverse direction on the bra space, and then you need the left side Q_0 to be present since it is then the first to act! So basically our two "protectors" allow us to have the function $(E_a^0 - H_0)^{-1}$: $(\mathcal{E}_a^0)^\perp \rightarrow (\mathcal{E}_a^0)^\perp$ exist in the middle, and this inverse does exist, as we just showed !

It is amazing how much is going on here that Messiah glosses over in the usual writer's need to minimize pages spent on obscure topics in a textbook.

g. The Perturbation Theory Equation Set

We must now look at the main perturbation theory equation set which is Schiff 31.4 or Messiah 16.7 page 687. In my Schiff notes I give an exact derivation of the equation set and I write it in this way

$$(H_0 - E_m)\ \psi^{(m)}_s = (W^{(m)}_1 - H')\ \psi^{(m)}_{s-1} + \Sigma_{j=2,3..s}\ W^{(m)}_j\ \psi^{(m)}_{s-j} \qquad s = 1,2,3...$$

so

$$(H_0 - E_m)\ \psi^{(m)}_0 = 0 \qquad s = 0$$

$$(H_0 - E_m)\ \psi^{(m)}_1 = (W^{(m)}_1 - H')\ \psi^{(m)}_0 \qquad s = 1$$

$$(H_0 - E_m)\ \psi^{(m)}_2 = (W^{(m)}_1 - H')\ \psi^{(m)}_1 + W^{(m)}_2\ \psi^{(m)}_0 \qquad s = 2$$

$$(H_0 - E_m)\ \psi^{(m)}_3 = (W^{(m)}_1 - H')\ \psi^{(m)}_2 + W^{(m)}_2\ \psi^{(m)}_1 + W^{(m)}_3\ \psi^{(m)}_0 \qquad s = 3$$

where each value of s is an equality for the power λ^s in the equation $(H+\lambda H')\psi = E\psi$ where we expand both ψ and E in λ. Here is a translation of the above into Messiah notation:

$(H_0 - E_a^0)\,|s\rangle = (\varepsilon_1 - V)\,|s\text{-}1\rangle + \Sigma_{j=2,3..s}\,\varepsilon_j\,|s\text{-}j\rangle$ s = 1,2,3...

so

$(H_0 - E_a^0)\,|0\rangle = 0$ s = 0

$(H_0 - E_a^0)\,|1\rangle = (\varepsilon_1 - V)\,|0\rangle$ s = 1

$(H_0 - E_a^0)\,|2\rangle = (\varepsilon_1 - V)\,|1\rangle + \varepsilon_2\,|0\rangle$ s = 2 (*)

$(H_0 - E_a^0)\,|3\rangle = (\varepsilon_1 - V)\,|2\rangle + \varepsilon_2\,|1\rangle + \varepsilon_3\,|0\rangle$ s = 3

$(H_0 - E_a^0)\,|4\rangle = (\varepsilon_1 - V)\,|3\rangle + \varepsilon_2\,|2\rangle + \varepsilon_3\,|1\rangle + \varepsilon_4\,|0\rangle$ s = 4

$(H_0 - E_a^0)\,|5\rangle = (\varepsilon_1 - V)\,|4\rangle + \varepsilon_2\,|3\rangle + \varepsilon_3\,|2\rangle + \varepsilon_4\,|1\rangle + \varepsilon_5\,|0\rangle$ s = 5

where I show lots of equations to make the pattern clear. You can see the benefit of Messiah's notation in that things are compacted down very nicely. State |0> is some unperturbed eigenstate of H_0 that lies inside $\mathcal{E}_a^0$ (see s=0 equation above).

WARNING #1: In our write-up here, we now have two distinct meanings for the notation |s>. In our discussion earlier on projection operators, |s> was an arbitrary eigenstate of H_0 $|s\rangle = E_n^0\,|s\rangle$. But in the above perturbation expansion, |s> refers to the λ^s order correction of some H eigenstate state u_n. We might expand Messiah's notation to |s; n> to mean the s^{th} correction to the state |n>. Reader beware!

WARNING #2. This state |0> = |0; n> we have said is an eigenstate of H_0 with energy E_a^0, that is what the s=0 equation above says. BUT, **it is not just any eigenstate of H_0** !! This is a potential pitfall if you don't understand why. The state |0; n> is one of the special eigenstates of H_0 within $\mathcal{E}_a^0$ which is the λ = 0 component of a state we might just call |n_full> which solves $H\,|n\rangle = E_n\,|n\rangle$, where now H includes the perturbation and E_n is the exact energy to all orders, and |n_full> is the exact state to all orders. So in the above set of equations, if you start off with some arbitrary spanning set of basis states |r> that span $\mathcal{E}_a^0$, it is very unlikely that the state |r> will be a legal state |0;n> for the perturbation equations shown above! You have to somehow *discover* what the legal states |0; n> really are ! .

While we are here, suppose we close from the left with a basis bra <r| from the degenerate subspace $\mathcal{E}_a^0$. We then get,

$0 = \langle r|\,(\varepsilon_1 - V)\,|s\text{-}1;n\rangle + \Sigma_{j=2,3..s}\,\varepsilon_j\,\langle r|\,s\text{-}j;n\rangle$ s = 1,2,3...

$0 = \langle r|\,(\varepsilon_1 - V)\,|s\text{-}1;n\rangle + \Sigma_{j=2,3..s-1}\,\varepsilon_j\,\langle r|\,s\text{-}j;n\rangle + \varepsilon_s\langle 0;r|\,0;n\rangle$ s = 1,2,3...

so

$0 = 0$ s = 0

$0 = \langle r|\,(\varepsilon_1 - V)\,|0;n\rangle$ s = 1

$0 = \langle r|\,(\varepsilon_1 - V)\,|1;n\rangle + \varepsilon_2\langle r|0;n\rangle$ s = 2

$0 = \langle r|\,(\varepsilon_1 - V)\,|2;n\rangle + \varepsilon_2\langle r|1;n\rangle + \varepsilon_3\langle r|\,0;n\rangle$ s = 3

$0 = \langle r|\,(\varepsilon_1 - V)\,|3;n\rangle + \varepsilon_2\langle r|2;n\rangle + \varepsilon_3\langle r|1;n\rangle + \varepsilon_4\langle r|\,0;n\rangle$ s = 4

$0 = \langle r|\,(\varepsilon_1 - V)\,|4;n\rangle + \varepsilon_2\langle r|3;n\rangle + \varepsilon_3\langle r|2;n\rangle + \varepsilon_4\langle r|1;n\rangle + \varepsilon_5\langle r|\,0;n\rangle$ s = 5

and as just noted, we cannot replace <r| 0;n> with $\delta_{r,n}$ since | 0;n> is in general a lincomb of the basis states |r> in $\mathcal{E}_a^0$. In the general degenerate case, I don't think there is much one can do with the above set of equations.

h. Energy Equations for the Non-degenerate Case. Now, *in the special case* that $\mathcal{E}_a^0$ is non-degenerate, we can identify | 0;n> = |r> because there is only one state in $\mathcal{E}_a^0$. Then we can replace <r|0;n> = 1. Moreover, factors like <r|1;n > = 0 due to the tricky method of normalization, so things simplify a lot:

$0 = \langle 0;n| (\varepsilon_1 - V) |s-1;n\rangle + \varepsilon_s$ s = 1,2,3...

so

$0 = \langle 0;n| (\varepsilon_1 - V) |0;n\rangle = \langle 0;n| (- V) |0;n\rangle + \varepsilon_1$ s = 1

$0 = \langle 0;n| (- V) |1;n\rangle + \varepsilon_2$ s = 2

$0 = \langle 0;n| (- V) |2;n\rangle + \varepsilon_3$ s = 3

$0 = \langle 0;n| (- V) |3;n\rangle + \varepsilon_4$ s = 4

$0 = \langle 0;n| (- V) |4;n\rangle + \varepsilon_5$ s = 5

All the equations have exactly the same form and we conclude that

$\varepsilon_s = \langle 0;n| V |s-1;n\rangle$ including $\varepsilon_1 = \langle 0;n| V |0;n\rangle = V_{nn}$

We see the result that each energy correction is determined by the state correction of the preceding order.

But, going down just this path, we don't have any formulas for the state corrections, so we cannot really go on to compute the higher energy corrections.

We now resume talking about the general degenerate case.

i. The Utility of Q_{a0} and solving the non-degenerate problem to all orders.

Now, back to the utility of Q_{a0}. So far, Q_{0a} has been just an amusing mathematical toy with some odd properties. What happens if we apply Q_{a0} to all these equations in set (*) in the previous section. Recall from just above our theorem that

$$Q_{0a} (E_a^0 - H_0) = Q_0$$

Thus, on the LHS we can replace the fairly complicated operator $(H_0 - E_a^0)$ by $- Q_0$. And on the RHS we know that Q_0 on the right end of Q_{0a} kills off the |0> state which we know lies in $\mathcal{E}_a^0$. So the above equations become

$-Q_0 |s\rangle = Q_{0a} (\varepsilon_1 - V) |s-1\rangle + \Sigma_{j=2,3..s} \varepsilon_j Q_{0a} |s-j\rangle$ s = 1,2,3...

$Q_0 |s\rangle = Q_{0a} V |s-1\rangle - \varepsilon_1 Q_{0a} |s-1\rangle - \Sigma_{j=2,3..s} \varepsilon_j Q_{0a} |s-j\rangle$ s = 1,2,3...

$Q_0 |s\rangle = Q_{0a} V |s-1\rangle - \Sigma_{j=1,3..s} \varepsilon_j Q_{0a} |s-j\rangle$ s = 1,2,3...

so

$Q_0 |1\rangle = Q_{0a} V |0\rangle$ s = 1 (**)

$Q_0 |2\rangle = Q_{0a} V |1\rangle - \varepsilon_1 Q_{0a} |1\rangle$ s = 2

$$Q_0\,|3\rangle = Q_{0a}V\,|2\rangle - \varepsilon_1 Q_{0a}\,|2\rangle - \varepsilon_2 Q_{0a}\,|1\rangle \qquad s = 3$$
$$Q_0\,|4\rangle = Q_{0a}V\,|3\rangle - \varepsilon_1 Q_{0a}\,|3\rangle - \varepsilon_2 Q_{0a}\,|2\rangle - \varepsilon_3 Q_{0a}\,|1\rangle \qquad s = 4$$
$$Q_0\,|5\rangle = Q_{0a}V\,|4\rangle - \varepsilon_1 Q_{0a}\,|4\rangle - \varepsilon_2 Q_{0a}\,|3\rangle - \varepsilon_3 Q_{0a}\,|2\rangle - \varepsilon_4 Q_{0a}\,|1\rangle \qquad s = 5$$

In general, each of these equations tells us something about the portion of the state correction |n> which lies in the space $(\mathcal{E}_a{}^0)^\perp$.

j. State Corrections for the Non-degenerate Case. Now *just for the moment*, suppose we were doing *non-degenerate* with the usual normalization. In this case, $Q_o|n\rangle = |n\rangle$ for n > 1.Then we get

$$|s\rangle = Q_{0a}\,V\,|s\text{-}1\rangle - \Sigma_{j=1,3..s}\,\varepsilon_j\;Q_{0a}\,|s\text{-}j\rangle \qquad s = 1,2,3...$$

$$|1\rangle = Q_{0a}V\,|0\rangle \qquad \text{// agrees with Messiah p 689 (14)} \qquad s = 1$$
$$|2\rangle = Q_{0a}V\,|1\rangle - \varepsilon_1 Q_{0a}\,|1\rangle \qquad s = 2$$
$$|3\rangle = Q_{0a}V\,|2\rangle - \varepsilon_1 Q_{0a}\,|2\rangle - \varepsilon_2 Q_{0a}\,|1\rangle \qquad s = 3$$
$$|4\rangle = Q_{0a}V\,|3\rangle - \varepsilon_1 Q_{0a}\,|3\rangle - \varepsilon_2 Q_{0a}\,|2\rangle - \varepsilon_3 Q_{0a}\,|1\rangle \qquad s = 4$$
$$|5\rangle = Q_{0a}V\,|4\rangle - \varepsilon_1 Q_{0a}\,|4\rangle - \varepsilon_2 Q_{0a}\,|3\rangle - \varepsilon_3 Q_{0a}\,|2\rangle - \varepsilon_4 Q_{0a}\,|1\rangle \qquad s = 5$$

and now we have *explicit formulas* for each state correction. We can then jam these states into our energy correction equation we found above which said $\varepsilon_s = \langle 0;r|V|s\text{-}1;r\rangle$ for our non-degenerate (now) state r.

k. Solution Algorithm for the Non-degenerate Case. So here is a viable algorithm for solving to all orders in this case: [each pair of computations can be done in either order]

for s = 1 to ∞ do begin
  compute $|s\rangle = Q_{0a}\,V\,|s\text{-}1\rangle - \Sigma_{j=1,3..s}\,\varepsilon_j\;Q_{0a}\,|s\text{-}j\rangle$
  compute $\varepsilon_s = \langle 0;n|\,V\,|s\text{-}1;n\rangle$
end

Here is the thing linearized for a bit:

	# terms	
$\|1\rangle = Q_{0a}V\,\|0\rangle$	1	s = 1
$\varepsilon_1 = \langle 0\|\,V\,\|0\rangle = V_{nn}$	1	
$\|2\rangle = Q_{0a}V\,\|1\rangle - \varepsilon_1 Q_{0a}\,\|1\rangle$	2	s = 2
$\varepsilon_2 = \langle 0\|\,V\,\|1\rangle$	1	
$\|3\rangle = Q_{0a}V\,\|2\rangle - \varepsilon_1 Q_{0a}\,\|2\rangle - \varepsilon_2 Q_{0a}\,\|1\rangle$	5	s = 3
$\varepsilon_3 = \langle 0\|\,V\,\|2\rangle$	2	
$\|4\rangle = Q_{0a}V\,\|3\rangle - \varepsilon_1 Q_{0a}\,\|3\rangle - \varepsilon_2 Q_{0a}\,\|2\rangle - \varepsilon_3 Q_{0a}\,\|1\rangle$	13	s = 4
$\varepsilon_4 = \langle 0\|\,V\,\|3\rangle$	5	
$\|5\rangle = Q_{0a}V\,\|4\rangle - \varepsilon_1 Q_{0a}\,\|4\rangle - \varepsilon_2 Q_{0a}\,\|3\rangle - \varepsilon_3 Q_{0a}\,\|2\rangle - \varepsilon_4 Q_{0a}\,\|1\rangle$	34	s = 5
$\varepsilon_5 = \langle 0\|\,V\,\|4\rangle$	13	

You can see that expressions are going to get very messy. I will write out some of the simpler ones:

$$|2> = Q_{0a}V\,Q_{0a}V\,|0> - \varepsilon_1\,Q_{0a}^2\,V\,|0>$$

$$|3> = Q_{0a}V\{\,Q_{0a}V\,Q_{0a}V\,|0> - \varepsilon_1\,Q_{0a}\,Q_{0a}V\,|0>\}$$
$$- \varepsilon_1\,Q_{0a}\,\{\,Q_{0a}V\,Q_{0a}V\,|0> - \varepsilon_1\,Q_{0a}\,Q_{0a}V\,|0>\} - \varepsilon_2\,Q_{0a}\,Q_{0a}V\,|0>$$

$$= Q_{0a}V\,Q_{0a}V\,Q_{0a}V\,|0> - \varepsilon_1\,Q_{0a}^2V\,|0> - \varepsilon_1\,Q_{0a}\,^2V\,Q_{0a}V\,|0> + \varepsilon_1^2\,Q_{0a}^3\,V\,|0> - \varepsilon_2\,Q_{0a}^2V\,|0>$$

so here are the 5 terms alluded to in the table above. We know that dim(Q_{0a}) = 1/energy, so the operator in each term above (and the term overall) is dimensionless, a way perhaps to check things. Each time there is a power of Q_{0a}, we are going to have a sum as shown in the examples below, so the first term on the last time implies three sums.

So, the reader perhaps now appreciates "the utility" of the operator Q_{a0} and sees why it was introduced. At least we have seen its use in the non-degenerate case.

l. Examples and a possible graphical language. Here are some examples showing the sums implied by the Q_{a0} factors:

$$|1;n> = Q_{0a}V\,|0;n> = \Sigma_{k\neq n}\,|0;k>\,(E_a^0 - E_k^0)^{-1}\,<0;k|\,V\,|0;n> = \Sigma_{k'\neq n}\,|0;k'>\,\{\,(E_a^0 - E_{k'}^0)^{-1}V_{k'n}\,\}$$

$$|2;n> = Q_{0a}(V - \varepsilon_1)\,|1;n> = \Sigma_{k'\neq n}\,|0;k'>\,(E_a^0 - E_{k'}^0)^{-1}<0;k'|\,(V - \varepsilon_1)\,|1;n>$$

$$= \Sigma_{k'\neq n}\,|0;k'>\,(E_a^0 - E_{k'}^0)^{-1}<0;k'\,|\,(V - \varepsilon_1)\,\{\,\Sigma_{k\neq n}\,|0;k>\,(E_a^0 - E_k^0)^{-1}V_{kn}\,\}$$

$$= \Sigma_{k',k\neq n}\,|0;k'>\,(E_a^0 - E_{k'}^0)^{-1}<0;k'\,|\,(V - \varepsilon_1)\,|0;k>\,(E_a^0 - E_k^0)^{-1}V_{kn}$$

$$= \Sigma_{k',k\neq n}\,|0;k'>\,(E_a^0 - E_{k'}^0)^{-1}\{\,V_{k'k} - V_{nn}\,\delta_{k',k}\}\,(E_a^0 - E_k^0)^{-1}V_{kn} \qquad \varepsilon_1 = V_{nn}$$

$$= \Sigma_{k'\neq n}\,|0;k'>\,\{\,\Sigma_{k\neq n}\,(E_a^0 - E_{k'}^0)^{-1}(E_a^0 - E_k^0)^{-1}V_{k'k}\,V_{kn} - (E_a^0 - E_{k'}^0)^{-2}\,V_{k'n}\,V_{nn}\,\}$$

where we can think of the thing in {..} as a coefficient of |0;k'> , namely, <0;k'| 2;n>. Thus we have computed that

$$<0;k'|\,1;n> = (E_a^0 - E_{k'}^0)^{-1}V_{k'n}$$

$$<0;k'|\,2;n> = -\,(E_a^0 - E_{k'}^0)^{-2}\,V_{k'n}\,V_{nn} + \Sigma_{k\neq n}\,(E_a^0 - E_{k'}^0)^{-1}(E_a^0 - E_k^0)^{-1}V_{k'k}\,V_{kn}$$

We can compare these with results from Schiff (from my raw notes on Chap 8)

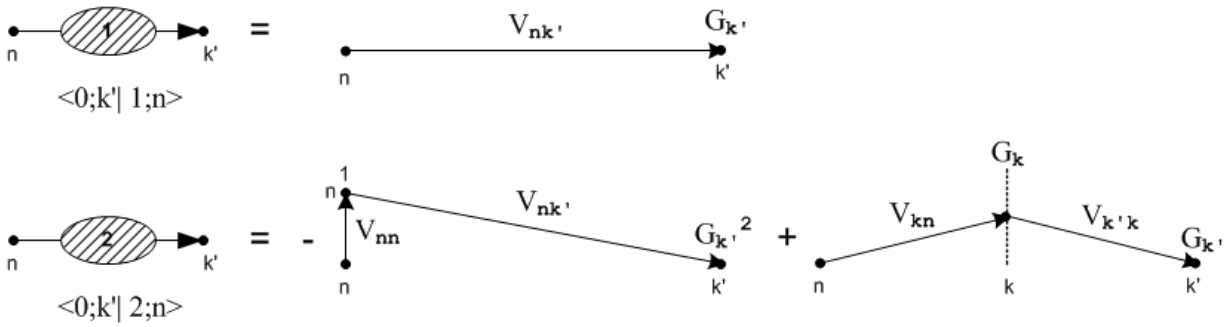
$$\psi^{(m)}_1 = \Sigma_{k\neq m}\,a^{(m)}_{k,1}\,u_k = \Sigma_{k\neq m}\,\{\,<k|\,H'\,|m>/(E_m - E_k)\,\}\,u_k$$

$$a^{(m)}_{k,2} = -<k|\,H'\,|m><m|H'|m>/\,(E_m - E_k)^2$$

$$+ \Sigma_{n\neq m} <k|\,H'\,|n><n|\,H'\,|m>/\,[(E_m - E_n)\,(E_m - E_k)] \qquad \textbf{// which is 31.13}$$

so I think both my results for |2;n> above is correct. You can get rid of some minus signs by negating the terms in the energy difference denominators.

One is very tempted to try to make some kind of Feynman like graph for this amplitude <0;k'| 2;n>, something like this: (remember that each V is of order λ)



In the degenerate case, we cannot carry out the above program because of the Q_0 factors on the LHS of all our perturbation equations (**) shown above, so we need a different plan.

Topic II. The Degenerate Case (698)

8. Elementary Theory (698)

Continuing the degenerate case, let's go back to our original equations

$(H_0 - E_a^0)\,|s\rangle = (\varepsilon_1 - V)\,|s\text{-}1\rangle + \Sigma_{j=2,3..s}\,\varepsilon_j\,|s\text{-}j\rangle$ s = 1,2,3...

so

$(H_0 - E_a^0)\,|0\rangle = 0$ s = 0

$(H_0 - E_a^0)\,|1\rangle = (\varepsilon_1 - V)\,|0\rangle$ s = 1

$(H_0 - E_a^0)\,|2\rangle = (\varepsilon_1 - V)\,|1\rangle + \varepsilon_2\,|0\rangle$ s = 2 (*)

$(H_0 - E_a^0)\,|3\rangle = (\varepsilon_1 - V)\,|2\rangle + \varepsilon_2\,|1\rangle + \varepsilon_3\,|0\rangle$ s = 3

$(H_0 - E_a^0)\,|4\rangle = (\varepsilon_1 - V)\,|3\rangle + \varepsilon_2\,|2\rangle + \varepsilon_3\,|1\rangle + \varepsilon_4\,|0\rangle$ s = 4

$(H_0 - E_a^0)\,|5\rangle = (\varepsilon_1 - V)\,|4\rangle + \varepsilon_2\,|3\rangle + \varepsilon_3\,|2\rangle + \varepsilon_4\,|1\rangle + \varepsilon_5\,|0\rangle$ s = 5

Finding the ε_1 eigenvalue problem.

Apply P_0 on the left (this is really P_{a0}). P_0 kills off the LHS's. Also, since we know |0> is in $\mathcal{E}_a^0$ (though we don't know the right linear combinations yet for such states |0>), we have $P_0|0\rangle = |0\rangle$. So we get this:

$0 = (\varepsilon_1 - V)\,|s\text{-}1\rangle + \Sigma_{j=2,3..s}\,\varepsilon_j\,|s\text{-}j\rangle$ s = 1,2,3...

so

$0 = 0$ s = 0

$0 = P_0\,(\varepsilon_1 - V)\,|0\rangle = \varepsilon_1\,|0\rangle - P_0 V\,|0\rangle$ s = 1

$0 = P_0 (\varepsilon_1 - V) |1\rangle + \varepsilon_2 |0\rangle$ s = 2

$0 = P_0 (\varepsilon_1 - V) |2\rangle + \varepsilon_2 P_0 |1\rangle + \varepsilon_3 |0\rangle$ s = 3

$0 = P_0 (\varepsilon_1 - V) |3\rangle + \varepsilon_2 P_0 |2\rangle + \varepsilon_3 P_0|1\rangle + \varepsilon_4 |0\rangle$ s = 4

$0 = P_0 (\varepsilon_1 - V) |4\rangle + \varepsilon_2 P_0 |3\rangle + \varepsilon_3 P_0 2\rangle + \varepsilon_4 P_0 |1\rangle + \varepsilon_5 |0\rangle$ s = 5

We now write out the s=1 equation which we see *is* the ε_1 eigenvalue problem:

$[P_0V] |0; n, \varepsilon_1\rangle = \varepsilon_{1,n} |0; n,\varepsilon_1\rangle$

Our states $|0; n,\varepsilon_1\rangle$ are thus eigenstates of the operator $[P_0V]$. Since P_0 and V are each Hermitian, so is the product, and we expect to have real eigenvalues and N eigenvectors for n = 1,2,...N where N is the dimension of our space $\mathcal{E}_a^0$.

Note: we could write the above as $P_0VP_0 |0\rangle = \varepsilon_1|0\rangle$ and we would then be in agreement with the first full sentence of Messiah's on page 699.

Express the ε_1 eigenvalue problem in matrix notation:

Let's close on the left with our initial set $\langle r|$ of $\mathcal{E}_a^0$ basis states to get

$\langle r| P_0V |0; n,\varepsilon_1\rangle = \varepsilon_{1,n} \langle r| 0; n,\varepsilon_1\rangle$

$\langle r| V P_0 |0; n,\varepsilon_1\rangle = \varepsilon_{1,n} \langle r |0; n,\varepsilon_1\rangle$ since P_0 does nothing to $\mathcal{E}_a^0$

Now expand the projection operator

$\Sigma_{r'}\langle r| V |r'\rangle\langle r'| 0; n,\varepsilon_1\rangle = \varepsilon_{1,n} \langle r | 0; n,\varepsilon_1\rangle$ // see **Messiah p 699 A**, he uses $\langle E_a^0\alpha|$ for $\langle r|$

$\Sigma_{r'} V_{rr'} \psi^{(n)}_{r'} = \varepsilon_{1,n} \psi^{(n)}_{r}$ $\psi^{(n)}_{r} = \langle r | 0; n,\varepsilon_1\rangle$

$V \boldsymbol{\psi}^{(n)} = \varepsilon_{1,n} \boldsymbol{\psi}^{(n)}$ $| 0; n,\varepsilon_1\rangle = \Sigma_{r\in\mathcal{E}a0} |r\rangle\langle r | 0; n,\varepsilon_1\rangle$

So this is a well-defined NxN matrix diagonalization problem which we can solve both for the eigenvalues and the eigenvectors $\boldsymbol{\psi}^{(n)}$. The secular equation says $\det(V- \varepsilon_{1,n}) = 0$ and tells us the eigenvalues. So we have our problem in full control to the point where we can determine the $| 0; n,\varepsilon_1\rangle$ and the first order energy corrections $\varepsilon_{1,n}$. Compare this to our computer program above for solving the whole problem. This is the first two steps. It could happen that some or even all of the $\varepsilon_{1,n}$ are degenerate and we will deal with that below.

We can regard the new eigenstates $| 0; n,\varepsilon_1\rangle$ as a unitary transformation of the original bases states $|r\rangle$ that spanned our subspace $\mathcal{E}_a^0$. Let's define

$U^{(1)}_{r,n} = \langle r | 0; n,\varepsilon_1\rangle$

$U^{(1)*}_{r,n} = \langle 0; n,\varepsilon_1| r\rangle = U^{(1)\dagger}_{n,r} = U^{(1)-1}_{n,r}$

$U^{(1)}$ will be a unitary matrix of all states are properly orthonormalized which we shall assume. Then we can say

$$| 0; n,\varepsilon_1\rangle = \Sigma_{r\in\mathcal{E}a0} \; |r\rangle\langle r | 0; n,\varepsilon_1\rangle = \Sigma_{r\in\mathcal{E}a0} \; U^{(1)}{}_{r,n} \; |r\rangle$$

$$\langle 0; n,\varepsilon_1| = \Sigma_{r\in\mathcal{E}a0} \; \langle 0; n,\varepsilon_1| r\rangle\langle r| = \Sigma_{r\in\mathcal{E}a0} \; U^{(1)-1}{}_{n,r} \langle r|$$

Thus unitary transformation is the matrix that diagonalizes V:

$$(U^{(1)-1} \; V \; U^{(1)})_{nn'} \; = \; \varepsilon_n \delta_{n,n'}$$

Note 1: It may be that some values of ε_1 have multiplicity > 1 so groups of states might still be degenerate at the ε_1 level. Within each group, we will assume we have carried out the GSO process so that we have a well defined set of N orthonormal states which we call $| 0; n,\varepsilon_1\rangle$. Each of these is then a certain linear combination of our original base states $|r\rangle$.

Note 2: Remember that the level 0 states k in $(\mathcal{E}_a{}^0)^\perp$ are orthogonal to all the $|r\rangle$ in $\mathcal{E}_a{}^0$ and are thus orthogonal to the diagonalizing states $| 0; n,\varepsilon_1\rangle$ as well. This NxN diagonalization problem does not involve those other states k in $(\mathcal{E}_a{}^0)^\perp$. However, as we shall see later, the state corrections do involve these other states.

Express the ε_1 eigenvalue problem as an operator equation.

Above we had (in simplified notation)

$$P_0 V|0\rangle = \varepsilon_1 \; |0\rangle \qquad\qquad [P_0 \; V] \; |0; n, \varepsilon_1\rangle = \varepsilon_{1,n} \; |0; n,\varepsilon_1\rangle$$

where the eigenvectors $|0\rangle$ all exist in $\mathcal{E}_a{}^0$. If we replace $|0\rangle$ with $P_0 \; |0\rangle$ on both sides, the resulting equation will then be true not just for the $|0\rangle$ states which span $\mathcal{E}_a{}^0$, but also for all other states, and thus we end up with an operator equation version of our eigenvalue problem

$$P_0 V \; P_0 \; = \varepsilon_1 \; P_0$$

This is a wonderful trick. In effect, *both sides* of this equation have "protectors" (filters) facing both left and right. Thus, this equation will be valid in both the bra space and the ket space when acting on any state! This is the beauty of using projectors.

Finding the ε_2 eigenvalue problem.

In the ε_1 EV problem we found a set of N states $|0; n\rangle$ with eigenvalues $\varepsilon_{1,n}$. These states are the level 0 components of eigenstates of the full H through first order (which means V is taken into account). Let's assume some number of these states N_1 are still degenerate with some ε_1 and let's focus on this group of states and ignore all the other states. The number N_1 could range anywhere from 1 to N. The space spanned by these vectors $|0; n,\varepsilon_1\rangle$ we could call $\mathcal{E}_a{}^{0(1)}$. All N_1 of these states have the same value for |1;

n> so they are degenerate both at the 0 level and at the 1 level of correction. But only certain linear combinations of the states |0; n,ε_1> will be the level 0 components of actual solutions of the full SE through second order. It is very unlikely that the $\mathcal{E}_a^{0(1)}$ "base states"
|0; n,ε_1> we obtain from the ε_1 EV problem are the right states! This is similar to how we said that <r| states which spanned $\mathcal{E}_a^0$ were unlikely to be the right states |0;n> which were level 0 components of full SE solutions. So we are going to discover an ε_2 eigenvalue problem which is going to tell us the proper states |0; n,ε_2> that are the right linear combinations of the |0; n,ε_1> states which will have well-defined values of ε_2 , which means they are eigenstates of the full H up through second order. Obviously we might find that some of these |0; n,ε_2> states are still degenerate. We would then sort of "recur" our algorithm here in a space $\mathcal{E}_a^{0(1)(1)}$, say, and look for an ε_3 eigenvalue problem to determine the right linear combinations of the |0; n,ε_2> states which are then eigenstates of H up through third order. And we could continue this process to any level. For now, let's just try to find the ε_2 level EV problem.

So, we define $P^{(1)} \subset P_0$ as the sub-projector for our space $\mathcal{E}_a^{0(1)}$. We can then write our s=2 perturbation equation after we apply $P^{(1)}$ to both sides, the result is this: [see ( ) above]

$$0 = P^{(1)}(\varepsilon_1 - V)\,|1> + \varepsilon_2\,|0> \qquad (1)$$

We also have our s=1 "Q_{a0} projected equation" [see ( ) above]

$$Q_0\,|1> = Q_{0a}V\,|0> \qquad (2)$$

In order for (1) to become an eigenvalue equation, we need to have the |1> be gone and somehow get a |0> in its place. For higher order, we will have the same type of problem. We want to use (2) to "reduce" (1), but as things stand, we cannot do it because we need a Q_0 in front of |1> which we don't have. This difficulty gets resolved by the discovery of the following operator equation which I will derive below:

$$P^{(1)}\,(\varepsilon_1 - V) = -\,P^{(1)} V\,Q_0 \qquad D'$$

which you see manages to make Q_0 appear on the right just where we need it to be! Then if we insert D' into (1) and then insert (2) into that result, we get

$$0 = P^{(1)}(\varepsilon_1 - V)\,|1> + \varepsilon_2\,|0> = -\,P^{(1)} V\,Q_0\,|1> + \varepsilon_2\,|0> = -\,P^{(1)} V\,Q_{0a}V\,|0> + \varepsilon_2\,|0>$$

$$\Rightarrow\ P^{(1)}(V\,Q_{0a}V)\,|0> = \varepsilon_2\,|0> \qquad (3)$$

and this *is* our ε_2 eigenvalue equation! Below we will show how to express it in matrix form, and how to also express it as an operator equation, but first we want to **derive D'** . Recall from above our first order eigenvalue equation expressed as an operator equation:

$$P_0 V P_0 = \varepsilon_1 P_0 \qquad (4)$$

Of we apply $P^{(1)}$ from the left on both sides, we are in effect restricting this equation when it acts on the bra space to the subspace $\mathcal{E}_a{}^{0(1)}$ -- we are certainly allowed to do that. Then $P^{(1)}P_0 = P^{(1)}$ from the obvious filtering property, and we end up with this restriction of the above operator equation:

$$P^{(1)} V P_0 = \varepsilon_1 P^{(1)} \qquad (5)$$

We now replace $P_0 = (1 - Q_0)$ to get our result D'

$$P^{(1)} V (1 - Q_0) = \varepsilon_1 P^{(1)} \quad => \quad P^{(1)} (\varepsilon_1 - V) = - P^{(1)} V Q_0 \qquad D'$$

Express the ε_2 eigenvalue problem in matrix notation:

We start with (3) above

$$P^{(1)} (V Q_{0a} V) |0; m,\varepsilon_2> = \varepsilon_{2,m} |0; m,\varepsilon_2>$$

Close from the left with our ε_1 level "basis states" $<0; m',\varepsilon_1|$

$$<0; m',\varepsilon_1| P^{(1)} (V Q_{0a} V) |0; m,\varepsilon_2> = \varepsilon_{2,m} <0; m',\varepsilon_1|0; m,\varepsilon_2>$$

$$<0; m',\varepsilon_1| (V Q_{0a} V) P^{(1)} |0; m,\varepsilon_2> = \varepsilon_{2,m} <0; m',\varepsilon_1|0; m,\varepsilon_2>$$

In the second equation, we repeated what we did in the ε_1 case, moving now $P^{(1)}$ to the right. Now expand the projector:

$$\Sigma_{m''=1,N1} <0; m',\varepsilon_1| (V Q_{0a} V) | 0;m'',\varepsilon_1><0;m'',\varepsilon_1 |0; m,\varepsilon_2> = \varepsilon_{2,m} <0; m',\varepsilon_1|0; m,\varepsilon_2>$$

We could regard this directly as a matrix equation

$$\Sigma_{m''=1,N1} (V Q_{0a} V)_{m'm''} \psi(m,\varepsilon_2)_{m''} = \varepsilon_{2,m} \psi(m,\varepsilon_2)_{m'}$$

but we have to go off and compute the matrix $V Q_{0a} V$ in the basis of $| 0;m'',\varepsilon_1>$ states. I am happier to have the subscripts on things like V and Q_{0a} be those of the original |r> basis, so let's go through some extra steps to achieve this goal.

So we need to replace the states $|0; m,\varepsilon_2>$ with sums of our original base states, and we quote from above making some symbol changes

$$| 0; m'',\varepsilon_1> = \Sigma_{r\in\mathcal{E}a0} |r><r | 0; m'',\varepsilon_1> = \Sigma_{r\in\mathcal{E}a0} |r> U^{(1)}{}_{r,m''}$$

$$<0; m',\varepsilon_1| = \Sigma_{r'\in\mathcal{E}a0} <0; m',\varepsilon_1| r'><r' | = \Sigma_{r\in\mathcal{E}a0} |r'> U^{(1)-1}{}_{m',r'}$$

Putting these in we get

$$\Sigma_{m''=1,N1} \Sigma_{r\in\mathcal{E}a0} \Sigma_{r'\in\mathcal{E}a0} U^{(1)-1}{}_{m',r'} (V Q_{0a} V)_{r'r} U^{(1)}{}_{r,m''} <0;m'',\varepsilon_1 |0; m,\varepsilon_2>$$

$$= \varepsilon_{2,m} \ \langle 0; m',\varepsilon_1|0; m,\varepsilon_2\rangle$$

Now think of our solution eigenvectors in this way,

$$\psi(m,\varepsilon_2)_{m''} = \langle 0;m'',\varepsilon_1 |0; m,\varepsilon_2\rangle$$

so we then have

$$\Sigma_{m''=1,N1} \ \Sigma_{r\in\mathcal{E}a0} \Sigma_{r'\in\mathcal{E}a0} \ U^{(1)-1}{}_{m',r'} (V\, Q_{0a} V)_{r'r} \ U^{(1)}{}_{r,m''} \psi(m,\varepsilon_2)_{m''} = \varepsilon_{2,m} \ \psi(m,\varepsilon_2)_{m'}$$

$$(U^{(1)-1} V\, Q_{0a} V\, U^{(1)}) \ \boldsymbol{\psi}(m,\varepsilon_2) = \varepsilon_{2,m} \boldsymbol{\psi}(m,\varepsilon_2)$$

As you can see, all the information from the ε_1 solution is needed [in the form of $U^{(1)}$] in order to solve the ε_2 problem. Things are pretty complicated, but at least we can see how we would do this computationally if we had to. The eigenvalues ε_2 come from

$$\det (U^{(1)-1} V\, Q_{0a} V\, U^{(1)} - \varepsilon_2) = 0$$

Express the ε_2 eigenvalue problem as an operator equation.

We start with the eigenvector equation from above

$$P^{(1)}(V\, Q_{0a} V) \ |0; m,\varepsilon_2\rangle = \varepsilon_{2,m} \ |0; m,\varepsilon_2\rangle$$

where the eigenvectors $|0\rangle$ all exist in $\mathcal{E}_a{}^{0(1)}$. If we replace $|0; m,\varepsilon_2\rangle$ with $P^{(1)} |0; m,\varepsilon_2\rangle$ on both sides, the resulting equation will then be true not just for the $|0; m,\varepsilon_2\rangle$ states which span $\mathcal{E}_a{}^{0(1)}$, but also for all other states, and thus we end up with an operator equation version of our eigenvalue problem

$$P^{(1)}(V\, Q_{0a} V)\, P^{(1)} = \varepsilon_1 \, P^{(1)}$$

This is a wonderful trick. In effect, *both sides* of this equation have "protectors" (filters) facing both left and right. Thus, this equation will be valid in both the bra space and the ket space when acting on any state! This is the beauty of using projectors.

Finding the ε_3 eigenvalue problem.

Flushed with a feeling of success at lower levels, let's try to go one more level and see what happens. So, we define $P^{(1,1)} \subset P^{(1)} \subset P_0$ as the sub-projector for our space $\mathcal{E}_a{}^{0(1,1)}$ of some dimension $N_{1,1}$. We can then write our s=3 perturbation equation after we apply $P^{(1,1)}$ to both sides, the result is this: (I have also copied down the modified s = 2 equation)

$$0 = P^{(1,1)}(\varepsilon_1 - V\,) |1\rangle + \varepsilon_2 |0\rangle \qquad (1a) \qquad s = 2$$

$$0 = P^{(1,1)} (\varepsilon_1 - V) |2> + \varepsilon_2 P^{(1,1)} |1> + \varepsilon_3 |0> \qquad (1b) \qquad s = 3$$

We also have our s=1 "Q_{a0} projected equations" [see ( ) above]

$$Q_0 |1> = Q_{0a} V |0> \qquad (2a) \qquad s = 1$$

$$Q_0 |2> = Q_{0a} V |1> - \varepsilon_1 Q_{0a} |1> \qquad (2b) \qquad s = 2$$

We are now faced with the problem of eliminating *both* |2> and |1> from (1b) above, and we have the same need to cause some Q_0 factors to "appear" on the right. Let's blindly tread down the same path as before, making small changes. We can write our ε_1 EV operator equation (still further restricted) as

$$P^{(1,1)} V P_0 = \varepsilon_1 P^{(1,1)} \qquad (5)$$

$$P^{(1,1)} V (1 - Q_0) = \varepsilon_1 P^{(1,1)} \quad => \quad P^{(1,1)} (\varepsilon_1 - V) = - P^{(1,1)} V Q_0 \qquad D'$$

which is our new version of D'. This looks promising and we insert it at once into (1b) to get

$$0 = - P^{(1,1)} V Q_0 |2> + \varepsilon_2 P^{(1,1)} |1> + \varepsilon_3 |0>$$

and then we use (2b) to get

$$0 = - P^{(1,1)} V Q_{0a} V |1> - \varepsilon_1 Q_{0a} |1>) + \varepsilon_2 P^{(1,1)} |1> + \varepsilon_3 |0>$$

and we are happy to see the state |2> gone. We can further say, using (2a),

$$Q_{0a} |1> = Q_{0a} Q_0 |1> = Q_{0a} Q_{0a} V |0> = Q_{0a}^2 V |0>$$

and then we have

$$0 = - P^{(1,1)} V (Q_{0a} V |1> - \varepsilon_1 Q_{0a}^2 V |0>) + \varepsilon_2 P^{(1,1)} |1> + \varepsilon_3 |0>$$

$$0 = - P^{(1,1)} V Q_{0a} V |1> + \varepsilon_2 P^{(1,1)} |1> + \varepsilon_3 |0> + \varepsilon_1 Q_{0a}^2 V |0>$$

$$0 = P^{(1,1)} (V Q_{0a} V + \varepsilon_2) |1> + \varepsilon_3 |0> + \varepsilon_1 Q_{0a}^2 V |0>$$

Now we need to concoct some way to get Q_0 on the right end for this first term. We do have one other weapon which is our ε_2 EV operator equation,

$$P^{(1)} (V Q_{0a} V) P^{(1)} = \varepsilon_1 P^{(1)}$$

which can restrict from just the left side as we did last time

$$P^{(1,1)} (V Q_{0a} V) P^{(1)} = \varepsilon_1 P^{(1,1)}$$

Now blindly continuing, replace $P^{(1)} = 1 - Q_0{}^{(1)}$ where we define a new version of Q_0 . Then

$$P^{(1,1)}(V\, Q_{0a} V)\,(1 - Q_0{}^{(1)}) = \varepsilon_1\, P^{(1,1)}$$

And let's not forget our friendly s=2 equation from above which we alter slightly

$$0 = P^{(1,1)}(\varepsilon_1 - V)\,|1\rangle + \varepsilon_2\, P^{(1,1)}\,|0\rangle$$

Mix these things together a bit and we have

$$P^{(1,1)}\,(V\, Q_{0a} V + \varepsilon_2) = P^{(1,1)}(V\, Q_{0a} V)\, Q_0{}^{(1)} + \varepsilon_1\, P^{(1,1)}$$

Now, I think we can concoct a new version of (2a) above that says

$$Q_0{}^{(1)}\,|1\rangle = Q_{0a}{}^{(1)} V\,|0\rangle \qquad\qquad (2a) \qquad\qquad s = 1$$

where $Q_{0a}{}^{(1)} = Q_0{}^{(1)}(E_a{}^0 - H_0)^{-1}\, Q_0{}^{(1)}$. Let's just guess that this works and see what happens. We then have for our tentative EV equation precursor,

$$0 = P^{(1,1)}\,(V\, Q_{0a} V + \varepsilon_2)\,|1\rangle + \varepsilon_3\,|0\rangle + \varepsilon_1\, Q_{0a}{}^2\, V\,|0\rangle$$

$$0 = \{\, P^{(1,1)}(V\, Q_{0a} V)\, Q_0{}^{(1)} + \varepsilon_1\, P^{(1,1)}\}\,|1\rangle + \varepsilon_3\,|0\rangle + \varepsilon_1\, Q_{0a}{}^2\, V\,|0\rangle$$

$$0 = P^{(1,1)}(V\, Q_{0a} V)\, Q_0{}^{(1)}|1\rangle + \varepsilon_1\, P^{(1,1)}\,|1\rangle + \varepsilon_3\,|0\rangle + \varepsilon_1\, Q_{0a}{}^2\, V\,|0\rangle$$

$$0 = P^{(1,1)}(V\, Q_{0a} V)\, Q_{0a}{}^{(1)} V\,|0\rangle + \varepsilon_1\, P^{(1,1)}\,|1\rangle + \varepsilon_3\,|0\rangle + \varepsilon_1\, Q_{0a}{}^2\, V\,|0\rangle$$

OK, I give up after a valiant effort. We still have some $|1\rangle$ left over in this equation, so it is not yet en EV equation.

Finding the ε_s eigenvalue problem.

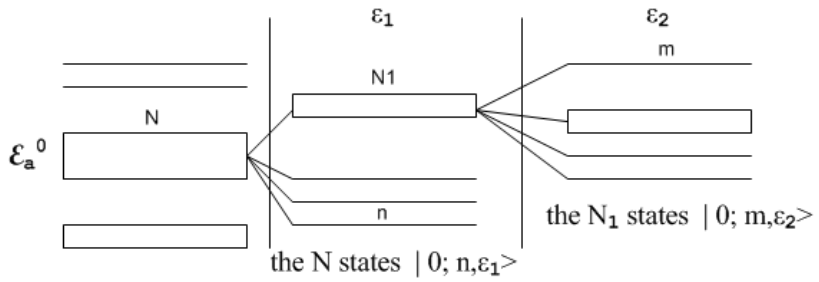
It is abundantly clear that you cannot continue down the same path as the order increases, because the complexity exponentiates and you have to somehow delicately thread your way exactly right through each level to find the EV equation. This is why we need a more systematic and organized attack on the problem, and Kato did this in 1949 and Messiah reported out his results.

P1. Finding the state corrections.

As outlined above, Messiah gets us to the point of an eigenvalue problem at each ε level, which of course has eigenvectors at that level, but he does not talk at all about how you would compute the state corrections like $|1\rangle$. Admittedly, it is usually the energies that are of most interest.

Computation of the |1> level state corrections.

Suppose a set of states were degenerate at the ε_0 level, but at the ε_1 level our "state n of interest" $|0; n,\varepsilon_1\rangle$ is non-degenerate. This state is marked in the following picture (ignore the ε_2 column for now)



Let the projector for this one state be $P^{(1)} = 1 - Q^{(1)}$. Then define

$$Q_{0a}^{(1)} \equiv Q_0^{(1)}(E_a^0 - H_0)^{-1}Q_0^{(1)} \qquad Q_0^{(1)} = \Sigma_{k\neq 1}\ |k\rangle\langle k|$$

This sum over k includes *all* states in $\mathcal{H}^0$ except our one state $|0; n,\varepsilon_1\rangle$. The sum does not *just* include states that were in the original degenerate group of N states in $\mathcal{E}_a^0$. So as a practical matter, the sum could to be computed as follows:

$$Q_0^{(1)} = \Sigma_{n'=1,N(n'\neq n)}\ |0; n',\varepsilon_1\rangle\langle 0; n',\varepsilon_1| + \Sigma_{k\in\mathcal{E}oa\perp}\ |k\rangle\langle k|$$

Here, the first sum includes all the other states in the ε_1 column of the above picture, and then the second sum include all the rest of the states in $(\mathcal{E}_a^0)^{\perp}$. Notice that the different elements of the first sum in general have different values for ε_1 (suggested by different vertical position in the picture).

In theory, we could have carried out our perturbation theory analysis on *all* states in the left column, so that the latter two columns of our picture would then be "fully populated". That requires of course a lot of work, because we have to solve the ε_1 level EV problem for all groups of degenerate states in the left column (in $\mathcal{E}_a^0$, $\mathcal{E}_b^0$, $\mathcal{E}_c^0$...) in order to fully populate the ε_1 column. But if we did all this work, then we could say

$$Q_0^{(1)} = \Sigma_{n'=all\ (n'\neq n)}\ |0; n',\varepsilon_1\rangle\langle 0; n',\varepsilon_1|$$

where now our sum would be over all "horizontal lines" in the ε_1 column that we get by tracking over all the states from the left column. Of course not all these lines are shown in our picture above. In other words, if we do all this work, then we have a new basis $|0; n,\varepsilon_1\rangle$ for the entire $\mathcal{H}$, and then we are just knocking one state out of our sum to get $Q_0^{(1)}$.

Further developing $Q_0^{(1)}$ using the first method above, we could of course use our expansions

$$|0; n',\varepsilon_1\rangle = \Sigma_{r'\in\mathcal{E}a0}\ |r'\rangle\langle r'|0; n',\varepsilon_1\rangle = \Sigma_{r'\in\mathcal{E}a0}\ U^{(1)}{}_{r',n'}|r'\rangle$$

$$\langle 0;\, n',\varepsilon_1| \;=\; \Sigma_{r\in\mathcal{E}a0}\; \langle 0;\, n',\varepsilon_1|\, r\rangle\langle r| \;=\; \Sigma_{r\in\mathcal{E}a0}\;\; U^{(1)-1}{}_{n',r}\; \langle r|$$

and then we would have

$$Q_0{}^{(1)} = \Sigma_{n'\neq n}\; \{\, \Sigma_{r'\in\mathcal{E}a0}\; U^{(1)}{}_{r',n'}|r'\rangle\}\{\, \Sigma_{r\in\mathcal{E}a0}\;\; U^{(1)-1}{}_{n',r}\; \langle r|\,\} + \Sigma_{k\in\mathcal{E}oa\perp}\, |k\rangle\langle k|$$

$$= \Sigma_{n'\neq n}\, \Sigma_{r'\in\mathcal{E}a0}\, \Sigma_{r\in\mathcal{E}a0}\, U^{(1)}{}_{r',n'}\, U^{(1)-1}{}_{n',r}\; |r'\rangle\langle r| \;\; + \;\Sigma_{k\in\mathcal{E}oa\perp}\, |k\rangle\langle k|$$

which is an interesting formula. It says that if you insist on working in "the original basis" (whatever it was), then in that basis $Q_0{}^{(1)}$ has lots of off diagonal elements in the first summation above. The form is a lot simpler (and diagonal) if you find out what the kets $|0;\, n,\varepsilon_1\rangle$ are, and then work in that basis!

This $Q_{0a}{}^{(1)}$ above fits my general projector sandwich model so it should follow that

$$Q_{0a}{}^{(1)}\; (E_a{}^0 - H_0) = Q_0{}^{(1)}$$

Now consider our s=1 equation

$$(H_0 - E_a{}^0)\; |1;\, n,\varepsilon_1\rangle \;\; = \;\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

and apply $Q_{0a}{}^{(1)}$ to both sides and get

$$Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

Close with $\langle 0;\, n',\varepsilon_1|$ where $n' \neq n$,

$$\langle 0;\, n',\varepsilon_1|\; Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = \langle 0;\, n',\varepsilon_1|\; Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

But we know that $\langle 0;\, n',\varepsilon_1|\; Q_0{}^{(1)} = \langle 0;\, n',\varepsilon_1|$, so write this as

$$\langle 0;\, n',\varepsilon_1|1;\, n,\varepsilon_1\rangle = \langle 0;\, n',\varepsilon_1|\; Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle \qquad\qquad n' \neq n$$

This tells us the projections of our state $|1;\, n,\varepsilon_1\rangle$ onto all the N-1 states $|0;\, n',\varepsilon_1\rangle$ for $n' \neq n$, and we know that the projection onto the one state $|0;\, n,\varepsilon_1\rangle$ is zero from our normalization condition. But we also have to worry about projections of our state $|1;\, n,\varepsilon_1\rangle$ onto all the other states k in $(\mathcal{E}_a{}^0)^{\perp}$. We can find these exactly as above, $Q_0{}^{(1)}$ of course "passes" these states through as well, so

$$\langle k|\; Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = \langle k|\; Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

$$\langle k\; |1;\, n,\varepsilon_1\rangle = \langle k|\; Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

Now we know the projection of $|1;\, n,\varepsilon_1\rangle$ onto ALL states in our problem, we can now construct the first order corrected state as follows:

$$|1; n,\varepsilon_1\rangle = \Sigma_{n'\neq n} |0; n',\varepsilon_1\rangle \langle 0; n',\varepsilon_1|1; n,\varepsilon_1\rangle + \Sigma_{k\in\mathcal{E}_{0a}\perp} |k\rangle \langle k|1; n,\varepsilon_1\rangle$$

$$= \Sigma_{n'\neq n} |0; n',\varepsilon_1\rangle \langle 0; n',\varepsilon_1| Q_{0a}^{(1)} (\varepsilon_1 - V) |0; n,\varepsilon_1\rangle + \Sigma_{k\in\mathcal{E}_{0a}\perp} |k\rangle \langle k| Q_{0a}^{(1)} (\varepsilon_1 - V) |0; n,\varepsilon_1\rangle$$

where

$$Q_0^{(1)} = \Sigma_{n'=1,N,\ n'\neq n} |0; n',\varepsilon_1\rangle \langle 0; n',\varepsilon_1| + \Sigma_{k\in\mathcal{E}_{0a}\perp} |k\rangle\langle k| = 1 - P_0^{(1)}$$

$$Q_{0a}^{(1)} = Q_0^{(1)} (E_a^0 - H_0)^{-1} Q_0^{(1)}$$

Within $\mathcal{E}_a^0$ we really need to work in the ε_1 basis $|0; n,\varepsilon_1\rangle$, otherwise the above equations expand out into a huge mess.

Computation of the |2> level state corrections.

We have this EV equation for the bundle of N_1 states degenerate in the ε_1 column

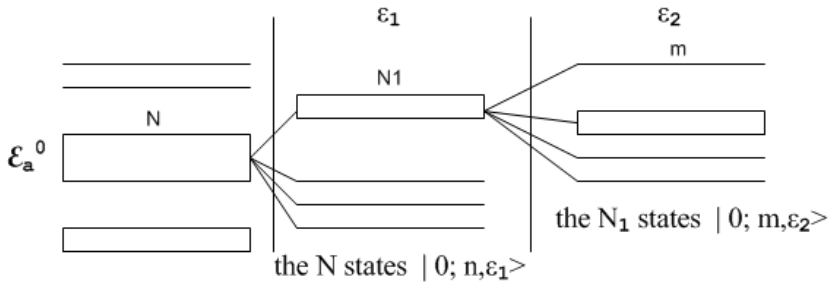
$$P^{(1)} (V\, Q_{0a} V) |0; m,\varepsilon_2\rangle = \varepsilon_2 |0; m,\varepsilon_2\rangle \qquad m = 1,2...N_1$$

$$\Sigma_{m''=1,N1} \langle 0; m',\varepsilon_1| (V\, Q_{0a} V) | 0;m'',\varepsilon_1\rangle\langle 0;m'',\varepsilon_1 |0; m,\varepsilon_2\rangle = \varepsilon_{2,m} \langle 0; m',\varepsilon_1|0; m,\varepsilon_2\rangle$$

Imagine that we solve this problem for the energies ε_2 and the coefficients $\langle 0; m',\varepsilon_1|0; m,\varepsilon_2\rangle$. We then know all about the kets in the right column (at least those of interest to us and shown in the figure)

$$|0; m,\varepsilon_2\rangle = \Sigma_{m'=1,N1} |0; m',\varepsilon_1\rangle \langle 0; m',\varepsilon_1|0; m,\varepsilon_2\rangle$$

They are just certain linear combinations of ε_1 level states $| 0;m,\varepsilon_1\rangle$ And suppose at this level, some state $|0; m,\varepsilon_2\rangle$ becomes a singlet. This appears as the top state on the right,



We can define a $P_0^{(1,1)}$ and corresponding Q_0 for this one state

$$Q_{0a}^{(1,1)} \equiv Q_0^{(1,1)} (E_a^0 - H_0)^{-1} Q_0^{(1,1)}$$

$$Q_0^{(1,1)} = \Sigma_{m'=1,N1\,(m'\neq m)} |0; m',\varepsilon_2\rangle\langle 0;m',\varepsilon_2|$$

$$+ \Sigma_{n=N1+1,N} |0; n,\varepsilon_1\rangle \langle 0; n,\varepsilon_1| + \Sigma_{k\in\mathcal{E}_{0a}\perp} |k\rangle\langle k|$$

It is worth discussing the various sums here. Because $P_0^{(1,1)}$ "passes" *only* the state $|0; m,\varepsilon_2\rangle$ (top right in our picture), we know that $Q_0^{(1,1)}$ must pass all *other* states. Now, this projector $Q_0^{(1,1)}$ includes three groups.

First, we need to include all the other states in the ε_2 rightmost column shown above. There are N_1-1 such states. Just to be able to include them means that we must know what they are! Luckily, we know what they are from the ε_2 level EV problem solution.

Second, we must include all the other states in the ε_1 column below the N1 degenerate group. Only when we include these states will we have included a full basis of $\mathcal{E}_a^0$. There are N - N_1 such states. Just to be able to include them means that we must know what *they* are! Luckily, we know what *they* are from the ε_1 level EV problem solution.

Third and last, we have to include the states in $(\mathcal{E}_a^0)^\perp$.

Reminder: everything in the picture is at the "0 level" in terms of state representations. The picture is just showing the right linear combinations of our initial 0 level states.

Now let's assume we have first solved the ε_1 EV problem for the bundle of N degenerate states in the left column, and that we have then solved the ε_2 EV problem for the bundle of N_1 still degenerate states in the middle problem. We now recall our s=2 perturbation equation

$$(H_0 - E_a^0)\,|2\rangle = (\varepsilon_1 - V)\,|1\rangle + \varepsilon_2\,|0\rangle \qquad s = 2 \quad (*)$$

and we use the fact that (we have seen this many times now, same idea over and over again)

$$Q_{0a}^{(1,1)}\,(E_a^0 - H_0) = Q_0^{(1,1)}$$

Then we have

$$Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle$$

We are now going to close this with various groups of <0| level states, and for each group, the $Q_{0(1,1)}$ on the LHS will vanish when we apply it to the left, since all states will be "other" states relative to $|0;m,\varepsilon_2\rangle$:

$$\langle 0, m', \varepsilon_2|\,Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle 0, m', \varepsilon_2\,|2; m,\varepsilon_2\rangle$$

$$= \langle 0, m', \varepsilon_2|\,Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,\langle 0, m', \varepsilon_2|\,Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle \qquad m' \neq m$$

$$\langle 0, n', \varepsilon_1|\,Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle 0, n', \varepsilon_1\,|2; m,\varepsilon_2\rangle$$

$$= \langle 0, n', \varepsilon_1\,|\,Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,\langle 0, n', \varepsilon_2\,|\,Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle \qquad n = N_1{+}1,N$$

$$\langle k|\,Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle k|2; m,\varepsilon_2\rangle$$

$$= \langle k | Q_{0a}^{(1,1)} (\varepsilon_1 - V) | 1; m,\varepsilon_2 \rangle + \varepsilon_2 \langle k | Q_{0a}^{(1,1)} | 0; m,\varepsilon_2 \rangle \qquad k \in (\mathcal{E}_a^0)^\perp$$

Now finally, using all these projection coefficients, we can construct our ε_2 level state correction:

$$|2,m,\varepsilon_2 \rangle = \Sigma_{m'=1,N1(m'\neq m)} |0; m',\varepsilon_2\rangle\langle 0, m', \varepsilon_2 |2; m,\varepsilon_2\rangle$$

$$+ \Sigma_{n=N1+1,N} |0; n,\varepsilon_1\rangle \langle 0; n,\varepsilon_1| 2; m,\varepsilon_2\rangle$$

$$+ \Sigma_{k\in\mathcal{E}oa\perp} |k\rangle\langle k| 2; m,\varepsilon_2\rangle$$

********** scraps **********

everything here is junk, all of yesterday's work was wrong. Typical.

Definition of $P^{(1)}$ and $Q^{(1)}$.

We want to define $P^{(1)}$ to project out only the state "n" in the above picture. The corresponding $Q^{(1)}$ is then given by

$$Q_0^{(1)} = \Sigma_{n'=1,N(n'\neq n)} |0; n',\varepsilon_1\rangle \langle 0; n',\varepsilon_1| + \Sigma_{k\in\mathcal{E}oa\perp} |k\rangle\langle k|$$

Here, the first sum includes all the other states in the ε_1 column of the above picture (just those drawn), and then the second sum include all the rest of the states in $(\mathcal{E}_a^0)^\perp$. Notice that the different elements of the first sum in general have different values for ε_1 (suggested by different vertical position of lines in the picture).

Note 1: In theory, we could have carried out our perturbation theory analysis on *all* states in the left column, so that the latter two columns of our picture would then be "fully populated". That requires of course a lot of work, because we have to solve the ε_1 level EV problem for all groups of degenerate states in the left column (in $\mathcal{E}_a^0$, $\mathcal{E}_b^0$, $\mathcal{E}_c^0$...) in order to fully populate the ε_1 column. But if we did all this work, then we could say

$$Q_0^{(1)} = \Sigma_{n'=all\ (n'\neq n)} |0; n',\varepsilon_1\rangle \langle 0; n',\varepsilon_1|$$

where now our sum would be over all "horizontal lines" in the ε_1 column that we get by tracking over all the states from the left column. Of course not all these lines are shown in our picture above. In other words, if we do all this work, then we have a new basis $|0; n,\varepsilon_1\rangle$ for the entire $\mathcal{H}$, and then we are just knocking one state out of our sum to get $Q_0^{(1)}$.

Note 2: Further developing $Q_0^{(1)}$ using the *first* method above, we could of course use our expansions

$$| 0; n',\varepsilon_1\rangle = \Sigma_{r'\in\mathcal{E}a0} |r'\rangle\langle r' | 0; n',\varepsilon_1\rangle = \Sigma_{r'\in\mathcal{E}a0} U^{(1)}_{r',n'} |r'\rangle$$

$$\langle 0;\, n',\varepsilon_1| \;=\; \Sigma_{r\in\mathcal{E}a0}\; \langle 0;\, n',\varepsilon_1|\, r\rangle\langle r\,| \quad =\; \Sigma_{r\in\mathcal{E}a0}\;\; U^{(1)-1}{}_{n',r}\; \langle r|$$

and then we would have

$$Q_0{}^{(1)} = \Sigma_{n'\neq n}\; \{\, \Sigma_{r'\in\mathcal{E}a0}\; U^{(1)}{}_{r',n'}|r'\rangle\}\{\, \Sigma_{r\in\mathcal{E}a0}\;\; U^{(1)-1}{}_{n',r}\; \langle r|\,\} + \Sigma_{k\in\mathcal{E}oa\perp}\, |k\rangle\langle k|$$

$$= \Sigma_{n'\neq n}\, \Sigma_{r'\in\mathcal{E}a0}\, \Sigma_{r\in\mathcal{E}a0}\, U^{(1)}{}_{r',n'}\, U^{(1)-1}{}_{n',r}\; |r'\rangle\langle r| \quad + \;\Sigma_{k\in\mathcal{E}oa\perp}\, |k\rangle\langle k|$$

which is an interesting formula. It says that if you insist on working in "the original basis" (whatever it was), then in that basis $Q_0{}^{(1)}$ has lots of off diagonal elements in the first summation above. The form is a lot simpler (and diagonal) if you find out what the kets $|0;\, n,\varepsilon_1\rangle$ are, and then work in that basis!

Definition of $Q_{0a}{}^{(1)}$.

In my first go at this, I tried using $Q_{0a}{}^{(1)} \equiv Q_0{}^{(1)}(E_a{}^0 - H_0)^{-1}Q_0{}^{(1)}$, but then I realized that this does not work and is singular because we don't have full Q_0 "protection". For example, if we apply the above to some state $|0;\, n',\varepsilon_1\rangle$ with $n' \neq n$, we get $(E_a{}^0 - H_0)^{-1}Q_0{}^{(1)}\; |0;\, n',\varepsilon_1\rangle = (E_a{}^0 - H_0)^{-1}|0;\, n',\varepsilon_1\rangle = \infty$ since $|0;\, n',\varepsilon_1\rangle$ is a linear combination of states which span $\mathcal{E}_a{}^0$. A better candidate is this:

$$Q_{0a}{}^{(1)} \equiv Q_0{}^{(1)}Q_0\, (E_a{}^0 - H_0)^{-1}\, Q_0Q_0{}^{(1)} \quad = Q_0{}^{(1)}Q_{0a}\, Q_0{}^{(1)}$$

This $Q_{0a}{}^{(1)}$ above fits my general projector sandwich model so it should follow that

$$Q_{0a}{}^{(1)}\; (E_a{}^0 - H_0) = Q_0{}^{(1)}$$

Now consider our s=1 equation

$$(H_0 - E_a{}^0)\; |1;\, n,\varepsilon_1\rangle \;=\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

and apply $Q_{0a}{}^{(1)}$ to both sides and get

$$Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = Q_{0a}{}^{(1)}\; (\varepsilon_1 - V\,)\; |0;\, n,\varepsilon_1\rangle$$

The ε_1 term vanishes because $Q_0{}^{(1)}\; |0;\, n,\varepsilon_1\rangle = 0$, so things simplify to

$$Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = -\, Q_{0a}{}^{(1)}V\; |0;\, n,\varepsilon_1\rangle$$

Close with $\langle 0;\, n',\varepsilon_1|$ where $n' \neq n$,

$$\langle 0;\, n',\varepsilon_1|\; Q_0{}^{(1)}\; |1;\, n,\varepsilon_1\rangle = -\, \langle 0;\, n',\varepsilon_1|\; Q_{0a}{}^{(1)}V\; |0;\, n,\varepsilon_1\rangle =$$

But we know that $\langle 0;\, n',\varepsilon_1|\; Q_0{}^{(1)} = \langle 0;\, n',\varepsilon_1|$, so write this as

$$\langle 0;\, n',\varepsilon_1 | 1;\, n,\varepsilon_1\rangle = \langle 0;\, n',\varepsilon_1 |\, Q_{0a}^{(1)} V\,) \,|0;\, n,\varepsilon_1\rangle \qquad\qquad n' \neq n$$

$$= \langle 0;\, n',\varepsilon_1 |\, Q_0^{(1)} (E_a^0 - H_0)^{-1} Q_0^{(1)} V\,) \,|0;\, n,\varepsilon_1\rangle = \langle 0;\, n',\varepsilon_1 |\, (E_a^0 - H_0)^{-1} Q_0^{(1)} V\,) \,|0;\, n,\varepsilon_1\rangle$$

$$= \Sigma_{r \in \mathcal{E}a0}\; U^{(1)-1}{}_{n',r}\, \langle r |\, (E_a^0 - H_0)^{-1} Q_0^{(1)} V\,) \,|0;\, n,\varepsilon_1\rangle \;\; = \text{diverges !!!!}$$

This tells us the projections of our state $|1;\, n,\varepsilon_1\rangle$ onto all the N-1 states $|0;\, n',\varepsilon_1\rangle$ for $n' \neq n$, and we know that the projection onto the one state $|0;\, n,\varepsilon_1\rangle$ is zero from our normalization condition. But we also have to worry about projections of our state $|1;\, n,\varepsilon_1\rangle$ onto all the other states k in $(\mathcal{E}_a^0)^{\perp}$. We can find these exactly as above, $Q_0^{(1)}$ of course "passes" these states through as well, so

$$\langle k |\, Q_0^{(1)} \,|1;\, n,\varepsilon_1\rangle = \langle k |\, Q_{0a}^{(1)} V \,|0;\, n,\varepsilon_1\rangle$$

$$\langle k \,|1;\, n,\varepsilon_1\rangle = \langle k |\, Q_{0a}^{(1)} V \,|0;\, n,\varepsilon_1\rangle \;=\; \langle k |\, Q_0^{(1)} (E_a^0 - H_0)^{-1} Q_0^{(1)} V \,|0;\, n,\varepsilon_1\rangle$$
$$= \langle k |\, (E_a^0 - H_0)^{-1} Q_0^{(1)} V \,|0;\, n,\varepsilon_1\rangle \;= (E_a^0 - E_k)^{-1}\, \langle k |\, Q_0^{(1)} V \,|0;\, n,\varepsilon_1\rangle$$
$$= (E_a^0 - E_k)^{-1}\, \langle k |\, V \,|0;\, n,\varepsilon_1\rangle$$

Now we know the projection of $|1;\, n,\varepsilon_1\rangle$ onto ALL states in our problem, we can now construct the first order corrected state as follows:

$$|1;\, n,\varepsilon_1\rangle \;=\; \Sigma_{n' \neq n} |0;\, n',\varepsilon_1\rangle\; \langle 0;\, n',\varepsilon_1 | 1;\, n,\varepsilon_1\rangle \;\; + \Sigma_{k \in \mathcal{E}oa\perp}\; |k\rangle\; \langle k \,|1;\, n,\varepsilon_1\rangle$$

$$= \Sigma_{n' \neq n} |0;\, n',\varepsilon_1\rangle \langle 0;\, n',\varepsilon_1 |\, Q_{0a}^{(1)} V \,|0;\, n,\varepsilon_1\rangle + \Sigma_{k \in \mathcal{E}oa\perp}\; |k\rangle \langle k |\, Q_{0a}^{(1)} V \,|0;\, n,\varepsilon_1\rangle$$

where

$$Q_0^{(1)} = \Sigma_{n'=1,N,\; n' \neq n}\; |0;\, n',\varepsilon_1\rangle \langle 0;\, n',\varepsilon_1| \;+ \Sigma_{k \in \mathcal{E}oa\perp} |k\rangle\langle k| \;\; = \; 1 - P_0^{(1)}$$

$$Q_{0a}^{(1)} \;= Q_0^{(1)} (E_a^0 - H_0)^{-1} Q_0^{(1)}$$

Within $\mathcal{E}_a^0$ we really need to work in the ε_1 basis $|0;\, n,\varepsilon_1\rangle$, otherwise the above equations expand out into a huge mess. In my "personal" degenerate perturbation theory notes I had this equation

$$\psi_{mi,1} \;= \{\; \Sigma_{j \neq i} B'_{ij,1}\; u_{mj} \;\} \oplus \Sigma_{k \neq m}\, B'_{ik,1}\, u_k \qquad\qquad \text{// n > 0, but have set n=1 in 3 placs}$$

and I kept having trouble finding the values for $B'_{ij,1}$. I was able to get the second coefficient set as

$$B'_{ik,1} \;=\; \langle u_k |\, V \,|u_{mi}\rangle / (E_m - E_k)$$

Computation of the |2> level state corrections.

We have this EV equation for the bundle of N_1 states degenerate in the ε_1 column

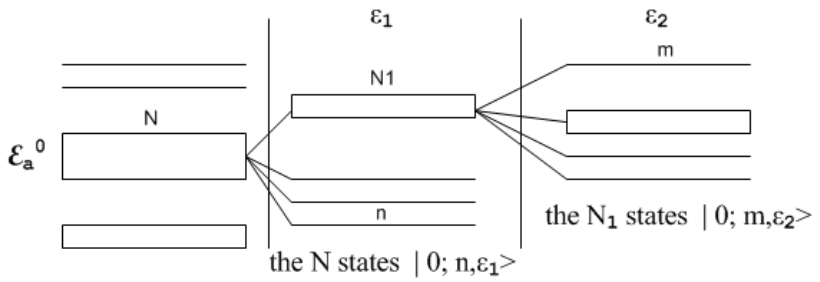
$P^{(1)}(V\,Q_{0a}V)\,|0;\,m,\varepsilon_2\rangle \;=\; \varepsilon_2\,|0;\,m,\varepsilon_2\rangle \qquad\qquad m = 1,2...N_1$

$\Sigma_{m''=1,N1}\;\langle 0;\,m',\varepsilon_1|\,(V\,Q_{0a}V)\,|\,0;m'',\varepsilon_1\rangle\langle 0;m'',\varepsilon_1\,|0;\,m,\varepsilon_2\rangle \;=\; \varepsilon_{2,m}\;\langle 0;\,m',\varepsilon_1|0;\,m,\varepsilon_2\rangle$

Imagine that we solve this problem for the energies ε_2 and the coefficients $\langle 0;\,m',\varepsilon_1|0;\,m,\varepsilon_2\rangle$. We then know all about the kets in the right column (at least those of interest to us and shown in the figure)

$|0;\,m,\varepsilon_2\rangle = \Sigma_{m'=1,N1}\;\;|0;\,m',\varepsilon_1\rangle\;\;\langle 0;\,m',\varepsilon_1|0;\,m,\varepsilon_2\rangle$

They are just certain linear combinations of ε_1 level states $|\,0;m,\varepsilon_1\rangle$ And suppose at this level, some state $|0;\,m,\varepsilon_2\rangle$ becomes a singlet. This appears as the top state on the right,



We can define a $P_0^{(1,1)}$ and corresponding Q_0 for this one state

$Q_{0a}^{(1,1)} \equiv Q_0^{(1,1)}\;(E_a^0 - H_0)^{-1}Q_0^{(1,1)}$

$Q_0^{(1,1)} = \Sigma_{m'=1,N1\,(m'\neq m)}\;\;|0;\,m',\varepsilon_2\rangle\langle 0;m',\varepsilon_2|$

$\quad + \;\Sigma_{n=N1+1,N}\;\;|0;\,n,\varepsilon_1\rangle\langle 0;\,n,\varepsilon_1| \quad + \quad \Sigma_{k\in\mathcal{E}_{oa}\perp}\,|k\rangle\langle k|$

It is worth discussing the various sums here. Because $P_0^{(1,1)}$ "passes" *only* the state $|0;\,m,\varepsilon_2\rangle$ (top right in our picture), we know that $Q_0^{(1,1)}$ must pass all *other* states. Now, this projector $Q_0^{(1,1)}$ includes three groups.

First, we need to include all the other states in the ε_2 rightmost column shown above. There are N_1-1 such states. Just to be able to include them means that we must know what they are! Luckily, we know what they are from the ε_2 level EV problem solution.

Second, we must include all the other states in the ε_1 column below the N1 degenerate group. Only when we include these states will we have included a full basis of $\mathcal{E}_a^0$. There are N - N_1 such states. Just to be able to include them means that we must know what *they* are! Luckily, we know what *they* are from the ε_1 level EV problem solution.

Third and last, we have to include the states in $(\mathcal{E}_a^0)^{\perp}$.

Reminder: everything in the picture is at the "0 level" in terms of state representations. The picture is just showing the right linear combinations of our initial 0 level states.

Now let's assume we have first solved the ε_1 EV problem for the bundle of N degenerate states in the left column, and that we have then solved the ε_2 EV problem for the bundle of N_1 still degenerate states in the middle problem. We now recall our s=2 perturbation equation

$$(H_0 - E_a^0)\,|2\rangle = (\varepsilon_1 - V)\,|1\rangle + \varepsilon_2\,|0\rangle \qquad s = 2 \quad (*)$$

and we use the fact that (we have seen this many times now, same idea over and over again)

$$Q_{0a}^{(1,1)}\,(E_a^0 - H_0) = Q_0^{(1,1)}$$

Then we have

$$Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\, Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle$$

We are now going to close this with various groups of <0| level states, and for each group, the $Q_{0\,(1,1)}$ on the LHS will vanish when we apply it to the left, since all states will be "other" states relative to $|0;m,\varepsilon_2\rangle$:

$$\langle 0, m', \varepsilon_2|\, Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle 0, m', \varepsilon_2\,|2; m,\varepsilon_2\rangle$$

$$= \langle 0, m', \varepsilon_2|\, Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,\langle 0, m', \varepsilon_2|\, Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle \qquad m' \neq m$$

$$\langle 0, n', \varepsilon_1|\, Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle 0, n', \varepsilon_1\,|2; m,\varepsilon_2\rangle$$

$$= \langle 0, n', \varepsilon_1\,|\, Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,\langle 0, n', \varepsilon_2\,|\, Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle \qquad n = N_1{+}1,N$$

$$\langle k|\, Q_0^{(1,1)}\,|2; m,\varepsilon_2\rangle = \langle k|2; m,\varepsilon_2\rangle$$

$$= \langle k\,|\, Q_{0a}^{(1,1)}\,(\varepsilon_1 - V)\,|1; m,\varepsilon_2\rangle + \varepsilon_2\,\langle k\,|\, Q_{0a}^{(1,1)}\,|0; m,\varepsilon_2\rangle \qquad k \in (\mathcal{E}_a^0)^{\perp}$$

Now finally, using all these projection coefficients, we can construct our ε_2 level state correction:

$$|2,m,\varepsilon_2\rangle = \Sigma_{m'=1,N1\,(m'\neq m)}\;|0; m',\varepsilon_2\rangle\langle 0, m', \varepsilon_2\,|2; m,\varepsilon_2\rangle$$

$$+\;\Sigma_{n=N1+1,N}\;|0; n,\varepsilon_1\rangle\langle 0; n,\varepsilon_1|\,2; m,\varepsilon_2\rangle$$

$$+\;\Sigma_{k\in\mathcal{E}_{0a}^{\perp}}\,|k\rangle\langle k|\,2; m,\varepsilon_2\rangle$$