Kato Meta Notes PhL 3.26.05

We are interested in the stationary-state perturbation problem for a group of N degenerate states of H_o. How exactly do you handle this situation to arbitrary order in λ^n ? The Kato method provides an answer, and also has some application to the non-degenerate case as well. This subject was amazingly complex on first reading, but now seems less so. All my raw notes are in three files called Kato Round 1,2,3, and this Meta Notes is the fourth and last file. You can see in the earlier rounds how I was confused and gradually understood things after several passes through the material. I never looked up the actual 1949 Kato paper and that probably would have made this job easier, but I would have had to trudge over to the U to get it.

Below we have first a contents of these Meta notes, then a Meta Meta review of them, then the actual Meta notes themselves. Page numbers here refer to the meta meta review.

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1. The Kato Method and Degeneracy. 1

2. The Kato Method Applied to a non-degenerate $\mathcal{E}_a^0$ 2

A. Comparison of the Kato state expansion with the Messiah special state expansion 3

B. Comments of Messiah at the start of his $g_a = 1$ section page 717. 3

C. Computing the energy corrections 3

1. The Kato Method and Degeneracy 4

Levels k = 1, k = 2, k = 3. 9

2. The Kato Method Applied to a non-degenerate $\mathcal{E}_a^0$ 11

A. Comparison of the Kato state expansion with the Messiah special state expansion 12

B. Comments of Messiah at the start of his $g_a = 1$ section page 717. 16

C. Computing the energy corrections 16

Appendix A 19

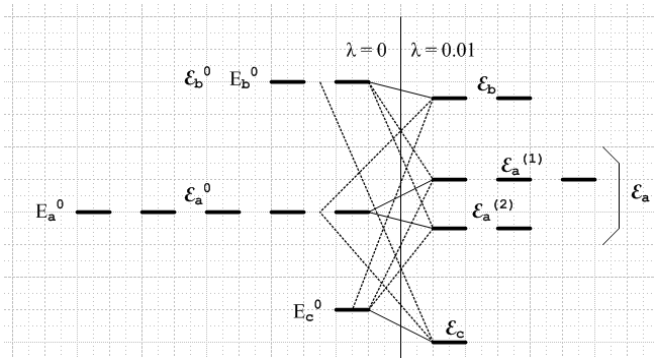
META META REVIEW (about 4 pages long)

1. The Kato Method and Degeneracy.

Here I review the Kato general method and show how it is used to resolve all situations involving degeneracy, including multiple levels of nested degeneracy. It is a complex problem. Kato was 1949. I am sure there are better methods on the market nowadays, but I think this was a great pioneering effort.

(0) The subspaces and projection operators associated with this problem are described.
For H one has S_i and P_i, while for H_0 one has S^0_i and P^0_i.

(1) The special dim=N subspaces $\mathcal{E}_a^0$ and $\mathcal{E}_a$ are highlighted. Kets of $\mathcal{E}_a^0$ are $|\psi_i ;0\rangle = |\varphi\rangle$.



Projectors which project onto these subspaces are called P_0 and P.
Each of these operators is 1:to:1 in the limited sense P: $\mathcal{E}_a^0 \rightarrow \mathcal{E}_a$ and P_0: $\mathcal{E}_a \rightarrow \mathcal{E}_a^0$.

(2) Any projector P_i for H can be represented as an integral around the pole at E_i:

$P_i = (2\pi i)^{-1} \oint_{\Gamma i} dz\ (z\text{-}H)^{-1}$ $\qquad\qquad$ $P = (2\pi i)^{-1} \int_{\Gamma a} dz\ (z\text{-}H)^{-1}$

On the right, the contour Γ_a encircles all the eigenenergy poles of space $\mathcal{E}_a$.

(3) A series simple expansion is developed for $(z\text{-}H)^{-1}$:
$(z\text{-}H)^{-1} = (z\text{-}H_0)^{-1} + (z\text{-}H_0)^{-1}\lambda V(z\text{-}H_0)^{-1} + (z\text{-}H_0)^{-1}\lambda V(z\text{-}H_0)^{-1}\lambda V(z\text{-}H_0)^{-1} + ...$
When installed in the above integral P and duly evaluated, we get a series expansion of P:
$P = P_0 + \lambda (P_0 V Q_{0a} + Q_{0a} V P_0) + \lambda^2$(six terms) $+ \lambda^3$ (lots of terms) + ...

(4) This section discusses the method used to evaluate the contour integrals for the above series.

(5) A similar expansion is developed for $B \equiv (H\text{-}E_a^0)P$. We arrive at an EV equation from the SE:
$B|\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P|\varphi_\alpha\rangle$ with $B = \Sigma_{i=1}\, \lambda^n B^{(n)}$ and $P = \Sigma_{i=0}\, \lambda^n P^{(n)}$

(6) To approximately solve the equation, wee keep only terms through some order λ^k.

(7) The problem is moved from $\mathcal{E}_a$ to $\mathcal{E}_a^0$ by applying P_0 to each side,
$P_0 B P_0 |\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P_0 P P_0 |\varphi_\alpha\rangle$ // both sides are kets in $\mathcal{E}_a^0$
which results in a reduction of the number of terms. If you use only k terms, the eigenkets of the EV equation are called $|\varphi_\alpha : k\rangle$, and vary (slightly) as you change k.

(8) For k=1 one gets $V|\varphi_\alpha : 1\rangle = \varepsilon_1 |\varphi_\alpha : 1\rangle$ and $\det[V - \varepsilon_1] = 0$ determines the N values of ε_1.

(9) For k=2 one gets $VQ_{a0}V|\varphi_\alpha : 2\rangle = \varepsilon_2 |\varphi_\alpha : 2\rangle$ and $\det[VQ_{a0}V - \varepsilon_2] = 0$.

(10) For k=3 one gets a true "generalized EV equation" and with an approximation one gets
$\{-VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V + VQ_{0a}VQ_{0a}V + VQ_{0a}^2V\}\, |\varphi_\alpha : 3\rangle = \varepsilon_3 |\varphi_\alpha : 3\rangle$
This shows how to handle all situations in our usual "picture" of nested degeneracy.
In general, one has to solve a generalized EV problem through order λ^k and this delivers the eigenenergies $\varepsilon_{12..k}$ of H through that order, as well as the eigenkets $|\varphi_\alpha : k\rangle$.

(11) Messiah only goes to k=2 in his non-Kato degeneracy analysis, results agree with Kato.

2. The Kato Method Applied to a non-degenerate $\mathcal{E}_a^0$

The basic EV equation $P_0 B P_0 |\varphi\rangle = (E_\alpha - E_a^0)\, P_0 P P_0 |\varphi\rangle$ is reviewed, and it is noted that $\mathcal{E}_a^0$ has one state $|\varphi\rangle$, and $\mathcal{E}_a$ has one state $|\psi\rangle$. If φ is normalized then it turns out that the action of our two basic projectors may be written as

$$P_0|\psi\rangle = |\varphi\rangle \quad \text{and} \quad P|\varphi\rangle = k\,|\psi\rangle \quad \text{where } k = \langle\varphi|P|\varphi\rangle = 1 + \lambda^2 C + \lambda^3 E + \ldots$$

As noted above, $P = P_0 + \lambda\,(P_0 V Q_{0a} + Q_{0a} V P_0) + \lambda^2(\text{six terms}) + \lambda^3\,(\text{lots of terms}) + \ldots$.
and this causes there to be no order λ term in k. The various constants like C and E can be evaluated by inserting the full expansion $P = \Sigma_{n=0}\,\lambda^n P^{(n)}$. It happens that $\langle\psi|\psi\rangle = 1/k$.

A. Comparison of the Kato state expansion with the Messiah special state expansion

The Kato method provides a natural state correction expansion

$$|\psi\rangle = \Sigma_{n=0}\,\lambda^n P^{(n)}|\varphi\rangle = |\varphi\rangle + \lambda\,P^{(1)}|\varphi\rangle + \ldots$$

This expansion is very much like my initial "personal notes" expansion which had this form,

$$\psi_{mi} = \{\, u_{mi} + \Sigma_j B_{ij}\, u_{mj} \,\} \oplus \Sigma_{k\neq m}\, B_{ik}\, u_k \qquad\qquad \psi_{mi} \in \mathcal{H}^{(m)} \oplus \mathcal{H}^{\perp}$$

where $B_{ij} = \Sigma_{n=0}\,\lambda^n B_{ij,n}\,|\varphi\rangle$ and same for B_{ik} , where $|\varphi\rangle = u_{mi}$. In my expansion, it is to be expected that some of the perturbation correction is proportional to u_{mi}. But this is a different expansion than the one which appears in Schiff and Messiah where we have to renormalize things to get

$$\psi'_{mi} = \{\, u_{mi} + \Sigma_{j\neq i} B'_{ij}\, u_{mj} \,\} \oplus \Sigma_{k\neq m}\, B'_{ik}\, u_k$$

where now none of the "corrections" are in the direction of u_{mi}. If we want to recast the Kato expansion so it looks like the Schiff/Messiah expansion, we have to do some rearrangement work on the series, and that is what this section is about. If the S/M expansion correction states are $|\psi\,;n\rangle$, then we find

$$|\psi\,;n\rangle = \text{coefficient of } \lambda^n \text{ in } \{\, \langle\varphi|\,\Sigma_{m=1}\,\lambda^m\, P^{(m)}|\varphi\rangle^{-1}\,[\,\Sigma_{k=1}\,\lambda^k\, P'^{(k)}|\varphi\rangle\,]\,\}$$

where we have to expand both sums sufficiently to extract the correct λ^n term. The prime indicates that subterms are thrown out which begin with P_0. We compare this state expansion to the iterative expansion given earlier by Messiah.

B. Comments of Messiah at the start of his $g_a = 1$ section page 717.

These comments seemed very mysterious on first reading, but are now clear, and here we document this simple fact.

C. Computing the energy corrections

The EV equation becomes $P_0 B P_0|\varphi\rangle = k(E_\alpha - E_a^0)|\varphi\rangle$ since $P_0 P P_0|\varphi\rangle = k|\varphi\rangle$. Thus.

$$\Sigma_{n=1}\lambda^n\varepsilon_n = (E_\alpha - E_a^0) = k^{-1}\langle\varphi|B|\varphi\rangle = \langle\varphi|\,(\Sigma_{m=1}\,\lambda^m\, P^{(m)})^{-1}|\varphi\rangle\,[\,\Sigma_{k=1}\,\lambda^k\, B^{(k)}|\varphi\rangle\,]\,\}$$

where again we have to extract a power in this sense

ε_n = coefficient of λ^n in $\{ \langle\varphi| (\Sigma_{m=1} \lambda^m P^{(m)})^{-1}|\varphi\rangle [\Sigma_{k=1} \lambda^k B^{(k)}|\varphi\rangle] \}$

For the lowest terms we find that $\varepsilon_1 = \langle\varphi| B^{(1)}|\varphi\rangle$, $\varepsilon_2 = \langle\varphi| B^{(2)}|\varphi\rangle$, but ε_3 is where we first see the mixing of the two power series in λ

$$\varepsilon_3 = \langle\varphi| B^{(3)}|\varphi\rangle - C\langle\varphi| B^{(1)}|\varphi\rangle \qquad C = -\langle\varphi| VQ_{0a}^2V|\varphi\rangle$$

Here, C is the first constant in $k = \langle\varphi|P|\varphi\rangle = 1 + \lambda^2C + \lambda^3E + \ldots$, so we then have

$$\begin{aligned}\varepsilon_3 &= \langle\varphi| B^{(3)}|\varphi\rangle + \langle\varphi| VQ_{0a}^2V|\varphi\rangle\langle\varphi| B^{(1)}|\varphi\rangle \\ &= \langle\varphi| B^{(3)}|\varphi\rangle + \langle\varphi| VQ_{0a}^2V|\varphi\rangle\langle\varphi|V|\varphi\rangle \\ &= \langle\varphi| B^{(3)}|\varphi\rangle + \langle\varphi| VQ_{0a}^2VP_0|V|\varphi\rangle\end{aligned}$$

This extra term is exactly what is needed to make this give the right answer for ε_3 as quoted in Messiah page 717 (74). So this is some evidence that the expression above is correct, though it does not appear in Messiah.

It is doubtless easier to compute the ε_n using the non-Kato method Messiah develops, which is this:

$$\varepsilon_n = \mathrm{tr}(B^{(n)}) = \langle\varphi| B'^{(n)}|\varphi\rangle$$

where prime means we knock out any one P_0 factor in each subterm of $B^{(n)}$. This is a more direct way to compute the energy corrections to arbitrary order. A clean and simple prescription.

In **Appendix A**, I took a quick (but not successful) shot at proving *directly* that these two methods for computing ε_n give the same results. Assuming I made no mistakes above, I know they are both correct. And I did show that they give the same results for ε_1, ε_2 and ε_3 where the last was non-trivial.

META REVIEW:

1. The Kato Method and Degeneracy

(0) The solution space of the full H can be partitioned into a set of **subspaces** S_i each of which has a **projection operator** P_i. Suppose there are m such subspaces (m could be infinite). We can then say

$$\mathcal{H} = \cup_{i=1,m} S_i \qquad 1 = \Sigma_{i=1,m} P_i$$

We have $H = H_0 + \lambda V$ and we could write a similar partition for H_0 as follows

$$\mathcal{H}^0 = \cup_{i=1,r} S^0_i \qquad 1 = \Sigma_{i=1,r} P^0_i$$

and we will use this idea a few subsections below. Here r is the number of subspaces S^0_i which partition $\mathcal{H}^0$ and we would in general expect to find $r \leq m$ since the perturbation tends to break degeneracy.

(1) In the Kato method for treating a degenerate situation, the N unperturbed states form a space called $\mathcal{E}_a^0$ where "a" just *labels* this group of states, since there are other eigenstates of H_0 including possible other degenerate groups. The space $\mathcal{E}_a^0$ is spanned by N kets $|\psi_i ;0\rangle = |\varphi\rangle$. The N kets $|\psi\rangle$ are the corresponding exact states of the full H and they span a space called $\mathcal{E}_a$. Kato's method does not deal with any "state expansions", but we could if we liked write one down, such as

$$|\psi\rangle = |\varphi\rangle + \Sigma_{n=1,\infty} \lambda^n |\psi_i ;n\rangle = \Sigma_{n=0,\infty} \lambda^n |\psi_i ;n\rangle$$

and this subject is addressed in a later section below.

The space $\mathcal{E}_a$ is the union of some of the subspaces S_i of H each of which has a projector P_i. There could be anywhere from 1 to N subspaces S_i in $\mathcal{E}_a$, depending on the degeneracy structure of the states in $\mathcal{E}_a$. Let's imagine there are n such subspaces. Then we can say [where $1 \le n \le N$]

$$\mathcal{E}_a = \cup_{i=1,n} S_i \qquad\qquad P \equiv \Sigma_{i=1,n} P_i$$

The projection operator P thus projects out of any ket that part belonging to the space $\mathcal{E}_a$, so we really have $P:\mathcal{H} \rightarrow \mathcal{E}_a$. If we restrict the domain to $\mathcal{E}_a^0$, we can talk about operator $P: \mathcal{E}_a^0 \rightarrow \mathcal{E}_a$ and this thing is 1-to-1 and therefore invertible with respect to this pair of spaces. Thus, for example, we can write any eigenstate $|\psi\rangle$ of H in the space $\mathcal{E}_a$ in the form $|\psi\rangle = P|\varphi\rangle$, where $|\varphi\rangle$ lies in $\mathcal{E}_a^0$. Specifically, we obtain $|\varphi\rangle$ as $|\varphi\rangle = P^{-1}|\psi\rangle$. This simple fact is crucial to the Kato development below.

The same argument can be made concerning P_0: $\mathcal{E}_a \rightarrow \mathcal{E}_a^0$ being 1-to-1 with respect to these two spaces and thus being invertible. This fact will also be used below. [In general we do not have $P^{-1} = P_0$ or vice versa.]

There is certainly nothing mysterious about P's definition as the projector onto $\mathcal{E}_a$.

The projector for the subspace $\mathcal{E}_a^0$ is called P_0 and will be used later. (that is, $P_0 \equiv P^0{}_a$ using the notation shown in (0) above).

(2) Kato goes on to produce a strange expansion of P in powers of λ, and this is much harder to understand. His first step is to express P as a contour integral. The following initial sequence of steps seems pretty clear: [book uses $G(z) = (z\text{-}H)^{-1}$ but we just write it all out here]

$$(z\text{-}H)^{-1}P_i = (z\text{-}E_i)^{-1}P_i \quad \Rightarrow \quad (z\text{-}H)^{-1} = \Sigma_i (z\text{-}E_i)^{-1}P_i \quad \Rightarrow \quad P_i = (2\pi i)^{-1} \oint_{\Gamma i} dz\, (z\text{-}H)^{-1}$$

The E_i are the eigenenergies of full H. Variable z is that of a "complex energy plane". So the rightmost equation tells us P_i as a function only of H and the eigenenergy E_i of S_i. Let's show that P_i given in this form really works:

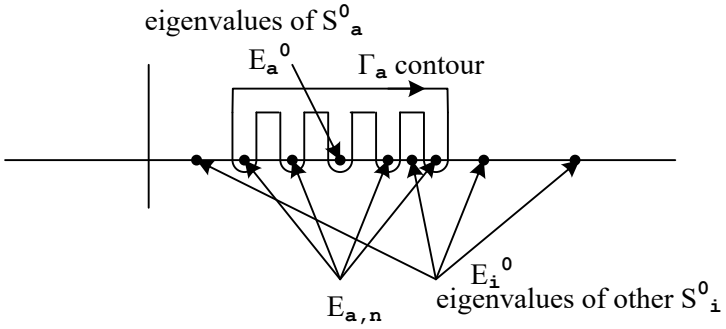
$$P_i|j\rangle = (2\pi i)^{-1} \oint_{\Gamma i} dz\, (z\text{-}H)^{-1}|j\rangle = (2\pi i)^{-1} \oint_{\Gamma i} dz\, (z\text{-}E_j)^{-1}|j\rangle$$

The integrand has a pole at E_j. If $|j> \in S_i$, the integral is 1 since the contour captures the pole. If $|j>$ is in some other S_j. the contour integral gives 0. So this in itself is really a derivation of our formula for P_i.

If we make the contour Γ_a encircle just the eigenenergies of the space $\mathcal{E}_a$ (but also the point E_a^0), we get a sum of the P_i for the subspaces S_i whose union is the space $\mathcal{E}_a$, and we have already defined this to be P, so we get

$$P = (2\pi i)^{-1} \int_{\Gamma a} dz\, (z-H)^{-1}$$

and here is a picture of this contour



(3) The next step is to expand $(z-H)^{-1}$ in powers of λ, and this will then provide an expansion of P in powers of λ which is our goal. The expansion of $(z-H)^{-1}$ starts out this way:

$$1 = (z-H_0)^{-1}(z-H_0) = (z-H_0)^{-1}(z-H+H-H_0) = (z-H_0)^{-1}(z-H) + (z-H_0)^{-1}(H-H_0)$$

$$(z-H)^{-1} = (z-H_0)^{-1} + (z-H_0)^{-1}(H-H_0)(z-H)^{-1} = (z-H_0)^{-1} + (z-H_0)^{-1}\lambda V (z-H)^{-1} \qquad (*)$$

The first line is trivial, and to get the second we right multiply the first line by $(z-H)^{-1}$. We thus end up with an integral equation of sorts for $(z-H)^{-1}$ which has the following formal series solution:

$$(z-H)^{-1} = \Sigma_{n=0}^{\infty} \lambda^n \{(z-H_0)^{-1}V(z-H_0)^{-1}V \ldots V(z-H_0)^{-1}\} \qquad \text{// n factors of V}$$

$$= (z-H_0)^{-1} + (z-H_0)^{-1}\lambda V(z-H_0)^{-1} + (z-H_0)^{-1}\lambda V(z-H_0)^{-1}\lambda V(z-H_0)^{-1} + \ldots$$

where the second form makes it clear this is a solution of (*). I think this kind of solution has some formal name like a Neumann series, but I forget right now. If we then insert this expansion of $(z-H)^{-1}$ into our integral representation of P, we get our expansion of P:

$$P = P_0 + \lambda (P_0 V Q_{0a} + Q_{0a} V P_0) + \lambda^2 (\text{six terms}) + \lambda^3 (\text{lots of terms}) + \ldots$$

(4) How were these terms evaluated? Looking at the first term, it must be true that

$$(2\pi i)^{-1} \int_{\Gamma a} dz\, (z-H_0)^{-1}\lambda V(z-H_0)^{-1} = \lambda (P_0 V Q_{0a} + Q_{0a} V P_0)$$

The way this evaluation is done is based on the following. First we can write each $(z\text{-}H_0)^{-1}$ factor as

$$(z\text{-}H_0)^{-1} = (z\text{-}E_a^0)^{-1}P_0 + \Sigma_{i\neq a}\,(z\text{-}E_i^0)^{-1}P^0{}_i \qquad \text{// sum over other } S_i^0$$

which is just a restatement of $(z\text{-}H)^{-1} = \Sigma_i\,(z\text{-}E_i)^{-1}P_i$ above when λ=0. The poles at $z = E_i^0$ lie outside the contour Γ_a as our picture shows. The only poles inside our contour are at $z = E_a^0$, so we may shrink our fancy contour to a simple circulation about the point $z = E_a^0$.

Kato then uses a Taylor series to expand the functions $(z\text{-}E_i^0)^{-1}$ about the point $z = E_a^0$ and the above becomes

$$(z\text{-}H_0)^{-1} = P_0/\,(z\text{-}E_a^0) + \Sigma_{n=1,\infty}\,(-1)^{n-1}\,(z\text{-}\,E_a^0)^{n-1}\,[\,\Sigma_{i\neq a}\,(E_a^0\text{-}\,E_i^0)^{-n}\,P_i^0]$$

$$= P_0/\,(z\text{-}E_a^0) + \Sigma_{n=1,\infty}\,(-1)^{n-1}\,(z\,\text{-}\,E_a^0)^{n-1}\,(Q_{0a})^n$$

where now the operator Q_{0a} suddenly appears! We know that Q_{0a} and Q_0 involve sums over states that are in the perp space of $\mathcal{E}_a^0$ and the perp space is the union of all the S_i^0 being summed by $\Sigma_{i\neq a}$, so this result is not too shocking. Details are given in the Round Three notes. This expression for $(z\text{-}H_0)^{-1}$ is certainly valid near the point $z = E_a^0$. The evaluation of all the Kato type integrals is now just a question of examining the interaction between the pole at $z = E_a^0$ and the various zeros at the same point.

(5) So, we have concocted the following series expansion for P:

$$P = P_0 + \lambda\,(P_0VQ_{0a} + Q_{0a}V\,P_0\,) + \lambda^2(\text{six terms}) + \lambda^3\,(\text{lots of terms}) + \ldots. = \Sigma_{n=0}\,\lambda^n P^{(n)}$$

A term in the set of terms for λ^n always has the form xVxVxV..Vx where there are N factors of V, and the x are either P_0 or Q_{0a}.

In a similar fashion, Kato provides an expansion for $B \equiv (H\text{-}E_a^0)P$ which is this

$$B = (H\text{-}E_a^0)P = 0 + \lambda(P_0VP_0) + \lambda^2(\text{three terms}) + \lambda^3\,(\text{lots of terms}) + \ldots. = \Sigma_{n=1}\,\lambda^n B^{(n)}$$

Now we said above that we can write any eigenstate $|\psi\rangle$ of H in the space $\mathcal{E}_a$ in the form $|\psi\rangle = P\,|\varphi\rangle$, where unique $|\varphi\rangle$ lies in $\mathcal{E}_a^0$. Thus consider an eigenstate of H called $|\psi_\alpha\rangle$. We can say

$$H|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle \qquad \text{// both sides are kets in } \mathcal{E}_a$$

and we know there exists a unique $|\varphi_\alpha\rangle$ in $\mathcal{E}_a^0$ such that

$$HP|\varphi_\alpha\rangle = E_\alpha P|\varphi_\alpha\rangle$$

We can then subtract $E_\alpha P|\varphi_\alpha\rangle$ from both sides to get

$$(HP - E_a^0P)\,|\varphi_\alpha\rangle = (E_\alpha - E_a^0)\,P|\varphi_\alpha\rangle$$

$B|\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P|\varphi_\alpha\rangle$ // both sides are kets in $\mathcal{E}_a$

We recognize $(E_\alpha - E_a^0)$ as the energy correction to all orders to the unperturbed energy E_a^0 and we know this is going to be order λ or higher. Now we can insert our Kato expansions for B and P on the two sides to get:

$$\Sigma_{i=1}\, \lambda^n B^{(n)}\, |\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, \Sigma_{i=0}\, \lambda^n\, P^{(n)}\, |\varphi_\alpha\rangle$$

(6) The Kato approximation method is to truncate the left side sum at some order i = k and the right side sum at some order k-1 so that both sides will have terms through λ^k :

$$[\, \lambda B^{(1)} + \lambda^2 B^{(2)} + .. \lambda^k B^{(k)}\,]\, |\varphi_\alpha\rangle = (E_\alpha - E_a^0)[\, 1 + \lambda P^{(1)} + ... + \lambda^{k-1}\, P^{(k-1)}\,]\, |\varphi_\alpha\rangle$$

where we used $P^{(0)} = P_0$ and $P_0\, |\varphi_\alpha\rangle = |\varphi_\alpha\rangle$. Since there is some operator on the right between the eigenvalue and the state, this is a "generalized eigenvalue equation" which I assume is solvable by people who know about these things (I do not).

(7) Kato actually uses a slightly different presentation. Due to the 1-1 connection between $\mathcal{E}_a$ and $\mathcal{E}_a^0$ provided by the projector P_0: $\mathcal{E}_a \rightarrow \mathcal{E}_a^0$, we can apply P_0 from the left to both sides of all our equations above and then our kets will all be in $\mathcal{E}_a^0$ instead of in $\mathcal{E}_a$. At the same time, we are free to extract a factor of P_0 on the right from the state $|\varphi_\alpha\rangle$. This leads to the alternative presentation:

$P_0 B P_0\, |\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P_0 P P_0 |\varphi_\alpha\rangle$ // both sides are kets in $\mathcal{E}_a^0$

$B''|\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P''|\varphi_\alpha\rangle$ // both sides are kets in $\mathcal{E}_a$

where we use a double prime to indicate that we have sandwiched P_0 around B and P. Our approximation above then becomes

$$P_0\, [\, \lambda B^{(1)} + \lambda^2 B^{(2)} + .. \lambda^k B^{(k)}\,]\, P_0\, |\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P_0\, [\, 1 + \lambda P^{(1)} + ... + \lambda^{k-1}\, P^{(k-1)}\,]\, P_0\, |\varphi_\alpha\rangle$$

This tends to simplify things because the leading (and also the trailing) P_0 allows for various terms to be removed since we have $P_0 Q_{0a} = Q_{0a} P_0 = 0$. In particular we have

$$P'^{(1)} = P_0\, P^{(1)} P_0 = P_0\, (P_0 V Q_{0a} + Q_{0a} V\, P_0) P_0 = 0$$

and various other terms simplify, so we can write out the first few terms on each side:

$$P_0\, [\, \lambda V + \lambda^2 V Q_{a0} V + .. \lambda^k B^{(k)}\,]\, P_0\, |\varphi_\alpha : k\rangle$$

$$= (E_\alpha - E_a^0)\, P_0\, [\, 1 - \lambda^2 V Q_{a0} V + ... + \lambda^{k-1}\, P^{(k-1)}\,]\, P_0\, |\varphi_\alpha : k\rangle$$

where our notation $|\varphi_\alpha : k\rangle$ reminds us that this eigenket solves this degree k problem. Do not confuse this with the eigenstate correction concept mentioned earlier. Here I used a colon separator.

For example, suppose you set k = 4 and suppose you somehow manage to solve this generalized eigenvalue equation for the N eigenkets $|\varphi_\alpha :4\rangle$ and for the eigenenergies $(E_\alpha - E_a^0)$. You then know these energies to order λ^4 (I think). You could then compute the eigenkets in $\mathcal{E}_a$ as $|\psi_\alpha\rangle = P|\varphi_\alpha\rangle$ where you would use the expansion for P through λ^4, and the solved-for eigenkets $|\varphi_\alpha\rangle$.

Levels k = 1, k = 2, k = 3.

(8) For k = 1 the approximation takes this form

$$P_0 [\lambda V] P_0 |\varphi_\alpha : 1\rangle = (E_\alpha - E_a^0) |\varphi_\alpha : 1\rangle$$

or just:

$$\lambda V |\varphi_\alpha : 1\rangle = (E_\alpha - E_a^0) |\varphi_\alpha : 1\rangle$$

This is in the N dimensional space $\mathcal{E}_a^0$ and the problem is then to diagonalize V within this space (only). The eigenvalues of this problem then tell us the eigenvalues of E_α to order λ. We usually write this equation as

$V |\varphi_\alpha : 1\rangle = \varepsilon_1 |\varphi_\alpha : 1\rangle$ $\qquad$ $\det[V - \varepsilon_1] = 0$ determines the N values of ε_1

(9) For k = 2 the approximation takes this form

$$[\lambda V + \lambda^2 V Q_{a0} V] |\varphi_\alpha : 2\rangle = (E_\alpha - E_a^0) |\varphi_\alpha : 2\rangle = (\lambda\varepsilon_1 + \lambda^2\varepsilon_2) |\varphi_\alpha : 2\rangle \equiv \varepsilon_{12} |\varphi_\alpha : 2\rangle$$

Although we have a messier operator to diagonalize, we still have a *non*-generalized EV problem which we think we know how to solve. The secular equation would be

$$\det [V + V Q_{a0} V - \varepsilon_{12}] = 0$$

which we could solve for our N values of ε_{12}, and then know $\varepsilon_2 = \varepsilon_{12} - \varepsilon_1$.

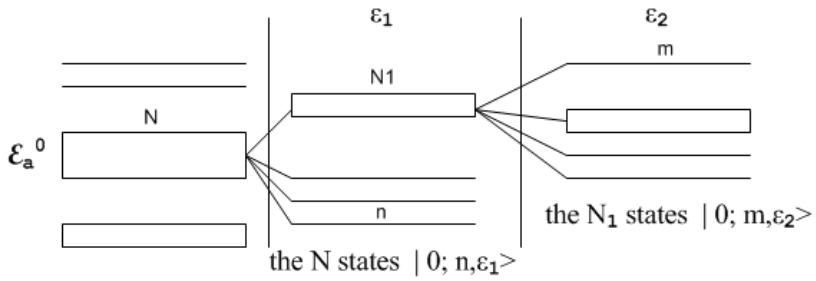
If we restrict this N dimensional problem to a M<N dimensional problem of a group of kets which remained degenerate in first order, we could *approximate* λV with the single eigenvalue of that first order problem, call it $[E_\alpha^{(1)} - E_a^0]$, then the above becomes

$$[\lambda^2 V Q_{a0} V] |\varphi_\alpha : 2\rangle = (E_\alpha - E_a^0 - [E_\alpha^{(1)} - E_a^0]) |\varphi_\alpha : 2\rangle = (E_\alpha - E_\alpha^{(1)}) |\varphi_\alpha : 2\rangle$$

and then solving this EV problem would give us E_α through second order λ^2 , and would give us some new states $|\varphi_\alpha : 2\rangle$ which are 'better' than those of the first order solution. We normally write this last equation then as

$V Q_{a0} V |\varphi_\alpha : 2\rangle = \varepsilon_2 |\varphi_\alpha : 2\rangle$ $\qquad$ $\det[V Q_{a0} V - \varepsilon_2] = 0$ determines the M values of ε_2

In the picture below, we show an example where M is written as N1



Of course this would also apply this approximation in the case M = 1 which would be our state "n" above, and in this case our equation is simply a 1x1 equation $VQ_{a0}V\ |\varphi : 2\rangle = \varepsilon_2\ |\varphi : 2\rangle$ and we then find that $\varepsilon_2 = \langle\varphi : 2|VQ_{a0}V\ |\varphi : 2\rangle$ which is the traditional non-degenerate state result Messiah p 694 (26) also shown as 717 (74). So to this order, for a state like n that started out degenerate and became solo at the first level, the ε_2 correction is that same as if he started out solo, provided you use the correct eigenstate.

(10) For k = 3 and higher, we have to worry about the operator on the RHS and we are in the realm of the *generalized* eigenvalue problem which is a little hazy to me. Here is what I got in my Round Three notes

$$\{ \lambda V + \lambda^2 VQ_{0a}V\ -\lambda^3 VQ_{0a}^2 VP_0 V - \lambda^3 VP_0 VQ_{0a}^2 V\ + \lambda^3 VQ_{0a}VQ_{0a}V \}\ |\varphi_\alpha : 3\rangle$$

$$= (E_\alpha - E_a^0)\{ 1- \lambda^2 VQ_{0a}^2 V\}\ |\varphi_\alpha : 3\rangle$$

Perhaps you could move the right side operator to the left saying

$$\{ 1- \lambda^2 VQ_{0a}^2 V\}^{-1} \approx \{ 1+ \lambda^2 VQ_{0a}^2 + O(\lambda^3)\ \}$$

to get this new LHS

$$\{ 1+ \lambda^2 VQ_{0a}^2 + O(\lambda^3)\ \}\{ \lambda V + \lambda^2 VQ_{0a}V\ -\lambda^3 VQ_{0a}^2 VP_0 V - \lambda^3 VP_0 VQ_{0a}^2 V\ + \lambda^3 VQ_{0a}VQ_{0a}V \}$$

$$= \{ \lambda V + \lambda^2 VQ_{0a}V\ -\lambda^3 VQ_{0a}^2 VP_0 V - \lambda^3 VP_0 VQ_{0a}^2 V\ + \lambda^3 VQ_{0a}VQ_{0a}V + \lambda^3\ VQ_{0a}^2 V\}$$

and then we have a regular eigenvalue equation

$$\{ \lambda V + \lambda^2 VQ_{0a}V\ -\lambda^3 VQ_{0a}^2 VP_0 V - \lambda^3 VP_0 VQ_{0a}^2 V\ + \lambda^3 VQ_{0a}VQ_{0a}V + \lambda^3\ VQ_{0a}^2 V\}\ |\varphi_\alpha : 3\rangle$$

$$= (E_\alpha - E_a^0)\ |\varphi_\alpha : 3\rangle\ = \varepsilon_{123}\ |\varphi_\alpha : 3\rangle$$

and we could write the secular equation as:

$$\det [V + VQ_{0a}V\ -VQ_{0a}^2 VP_0 V - VP_0 VQ_{0a}^2 V\ + VQ_{0a}VQ_{0a}V + VQ_{0a}^2 V - \varepsilon_{123}\ ] = 0$$

to get all N values of the energy corrections through third order, one for each of the N states.

If we still had a degenerate subspace $J \le M \le N$, we could approximate

$$\lambda V + \lambda^2 V Q_{0a} V \approx \lambda \varepsilon_1 + \lambda^2 \varepsilon_2$$

to get this equation:

$$\{-\lambda^3 V Q_{0a}^2 V P_0 V - \lambda^3 V P_0 V Q_{0a}^2 V + \lambda^3 V Q_{0a} V Q_{0a} V + \lambda^3 V Q_{0a}^2 V\} |\varphi_\alpha : 3\rangle = \lambda^3 \varepsilon_3 |\varphi_\alpha : 3\rangle$$

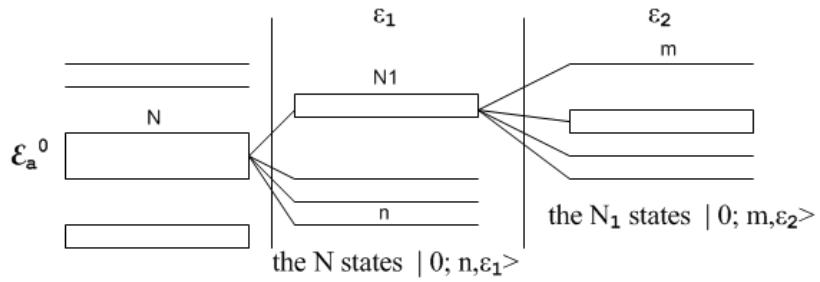
or

$$\{-V Q_{0a}^2 V P_0 V - V P_0 V Q_{0a}^2 V + V Q_{0a} V Q_{0a} V + V Q_{0a}^2 V\} |\varphi_\alpha : 3\rangle = \varepsilon_3 |\varphi_\alpha : 3\rangle$$

with a simpler secular equation

$$\det [-V Q_{0a}^2 V P_0 V - V P_0 V Q_{0a}^2 V + V Q_{0a} V Q_{0a} V + V Q_{0a}^2 V - \varepsilon_3] = 0$$

In terms of the above picture,



this last calculation would be applied to the group of states still degenerate in the ε_2 rightmost column. Think of these three bands as $N \ge M \ge J$. We could also apply this to solo state "m" in which case we get the result (ie, no need for a determinant)

$$\varepsilon_3 = \langle \varphi : 3| -V Q_{0a}^2 V P_0 V - V P_0 V Q_{0a}^2 V + V Q_{0a} V Q_{0a} V + V Q_{0a}^2 V |\varphi : 3\rangle$$

This result differs a little bit from the ε_3 correction of a state which begins life non-degenerate in the left column. The difference is that for that non-degenerate problem, the last term cancels the second term and we get Messiah page 717 (74). This is discussed below. [I might be wrong here]

(11) How does all this compare with Messiah's traditional degeneracy approach pp 698-700 ? He only discusses up to the λ^2 term. He uses the projection operator $P^{(1)}$ to reduce our N dimensional space to a smaller M dimensional space as we just did above. He ends up with $P^{(1)} V Q_{a0} V] |\varphi_\alpha\rangle = \varepsilon_2 P^{(1)} |\varphi_\alpha\rangle$ which is the same as our k=2 result above.

2. The Kato Method Applied to a non-degenerate $\mathcal{E}_a^0$

Everything done to this point allows for degeneracy N of the space $\mathcal{E}_a^0$. In the case that N = 1, there are certain dramatic simplifications. First, go back to our result above which said

$$B''|\varphi_\alpha\rangle = (E_\alpha - E_a^0)\, P''|\varphi_\alpha\rangle \qquad \text{// both sides are kets in } \mathcal{E}_a$$

If there is only one state $|\varphi\rangle$ in $\mathcal{E}_a^0$, then there is also only one state $|\psi\rangle$ in $\mathcal{E}_a$. Recall in deriving the above equation we claimed that *there exists* a unique $|\varphi\rangle$ in $\mathcal{E}_a^0$ such that $|\psi\rangle = P\,|\varphi\rangle$. No claim was made that either $|\psi\rangle$ or $|\varphi\rangle$ is normalized to unity. In the Messiah/Schiff (M/S) normalization scheme, we normalize ψ in a certain manner, and we want $|\varphi\rangle$ to have unit normalization. In this case, where we might be scaling both ψ and φ separately, we are really claiming that there exists a normalized $|\varphi\rangle$ and a specially normalized $|\psi\rangle$ such that $k\,|\psi\rangle = P|\varphi\rangle$ where k is some constant. This constant cancels on both sides of the above equation so we don't have to worry about it there.

Before examining the above eigenvalue equation and finding the eigenenergies, we digress first to talk about the "correction state expansion", something Messiah does not mention in the Kato section.

A. Comparison of the Kato state expansion with the Messiah special state expansion

Consider this expansion which we will call "the Kato state expansion", where I assume that the state $|\varphi\rangle$ is unit-normalized,

$$k|\psi\rangle = P|\varphi\rangle = \Sigma_{n=0}\, \lambda^n P^{(n)}|\varphi\rangle = |\varphi\rangle + \lambda\, Q_{0a}V|\varphi\rangle$$

$$+ \lambda^2 \{ (Q_{0a}VQ_{0a}V) - (Q_{0a}^2VP_0V + P_0VQ_{0a}^2V)\}\, |\varphi\rangle + \lambda^3 (..)|\varphi\rangle + \ldots$$

where we just insert the $P^{(n)}$ from above and simplify wherever possible (ie, delete right-side P_0 factors, and delete *terms* with Q_{0a} on the right). One might be tempted to equate this expansion term by term with the usual Messiah/Schiff (M/S) state expansion which is this

$$|\psi\rangle = |\varphi\rangle + \Sigma_{n=1,\infty}\, \lambda^n\, |\psi\,;n\rangle$$

but there is a *problem* in doing this. In the M/S expansion, we are supposed to assume the normalization conditions that $\langle\varphi|\psi\,;n\rangle = 0$ for n>0, and also $\langle\varphi|\varphi\rangle = 1$. In other words, none of the "correction states" $|\psi\,;n\rangle$ is supposed to have a component in $|\varphi\rangle$. Suppose we partition the eigenstates of H_o into our non-degenerate state of interest $|\varphi\rangle$ and all the other states we will just call $|k\rangle$. Then in the M/S expansion we are supposed to have correction states $|\psi\,;n\rangle$ which are linear combinations *only* of the states $|k\rangle$. But this, it turns out, is not true for the $P^{(n)}$ expansion above. For example, we see a term $-\lambda^2\, P_0VQ_{0a}^2V\,|\varphi\rangle$ appearing in this expansion. Due to the leftmost P_0, this correction state really has the form $\lambda^2\, C\,|\varphi\rangle$ where C is some constant, so this term is some multiple of $|\varphi\rangle$. We can compute:

$$C = -\langle\varphi|\, VQ_{0a}^2V|\varphi\rangle = -\Sigma_k\, (E_a^0 - E_k)^{-2}\, |V_{k0}|^2$$

So the Kato expansion becomes

$$k|\psi\rangle = (1 + \lambda^2 C)\,|\varphi\rangle + \lambda\, Q_{0a}V|\varphi\rangle$$

$$+ \lambda^2 \{ (Q_{0a}VQ_{0a}V) - (Q_{0a}^2VP_0V) \} |\varphi\rangle + \lambda^3 (..)|\varphi\rangle + ...$$

Any term that begins with a Q_{0a} cannot have a component in $|\varphi\rangle$. For example, let's look at the first λ^2 term and compute its projection onto $\langle\varphi|$.

$$\langle\varphi| \lambda^2 (Q_{0a}VQ_{0a}V) |\varphi\rangle = \lambda^2\langle\varphi| Q_0(E_a^0 - H_0)^{-1}Q_0VQ_{0a}V) |\varphi\rangle = 0$$

because $\langle\varphi| Q_0 = 0$, since Q_0 projects only onto the $|k\rangle$ states.

So, imagine that we write out the entire Kato expansion, and we compute all terms that begin with P_0 and find what multiple such terms are of $|\varphi\rangle$, and then we gather all these multiples up where we put the $\lambda^2 C$ shown above. Then we have this situation: (the state $|\varphi\rangle$ is normalized to 1)

$$k|\psi\rangle = (1 + \lambda^2 C + \lambda^3 C' + \lambda^4 C'' + ...) |\varphi\rangle + \lambda Q_{0a}V|\varphi\rangle$$

$$+ \lambda^2 \{ (Q_{0a}VQ_{0a}V) - (Q_{0a}^2VP_0V) \} |\varphi\rangle + \lambda^3 (..)|\varphi\rangle + ...$$

where in the main body of the expansion, there are no longer any terms beginning with P_0. Thus, all the above expansion terms respect the normalization condition $\langle\varphi|term\rangle = 0$. Let's then identify

$$k = (1 + \lambda^2 C + \lambda^3 C' + \lambda^4 C'' + ...)$$

Theorem: $k = \langle\varphi| P |\varphi\rangle$ and $\langle\psi|\psi\rangle = 1/k$; Messiah's use of the word "norm".

Note injected: Consider again

$$P|\varphi\rangle = \Sigma_{n=0} \lambda^n P^{(n)}|\varphi\rangle = |\varphi\rangle + \Sigma_{n=1} \lambda^n P^{(n)}|\varphi\rangle$$

This tells us that

$$\langle\varphi| P |\varphi\rangle = 1 + \langle\varphi| \Sigma_{n=1} \lambda^n P^{(n)}|\varphi\rangle = (1 + \lambda^2 C + \lambda^3 C' + \lambda^4 C'' + ...) = k$$

Thus, we can represent k in this manner

$$k = \langle\varphi| P |\varphi\rangle$$

and we can then say

$$|\psi\rangle = k^{-1}P|\varphi\rangle \Rightarrow \langle\psi|\psi\rangle = k^{-2}\langle\varphi|P\,P|\varphi\rangle = k^{-2}\langle\varphi| P|\varphi\rangle = k^{-1} = 1/\langle\varphi| P |\varphi\rangle$$

In Stakgold, the **"norm"** is defined as $||x|| = \langle x,x\rangle^{1/2}$ top of page 108 volume 1. But Messiah on page 165 defines his norm to be $N = \langle\psi|\psi\rangle$. Schiff and Saxon don't really use the word norm very much. So Messiah uses the word "norm" to be the length of a vector squared! I never noticed this before, and I think this is sort of a language misuse by Messiah.

But given Messiah's definition of the word "norm", it would be correct to say that the norm of the state $|\psi>$ is $1/<\varphi| P |\varphi>$ as he says on page 717.

And we then have

$$|\psi> = |\varphi> + \lambda k^{-1} Q_{0a} V|\varphi> +$$

$$\lambda^2 k^{-1} \{ (Q_{0a} V Q_{0a} V) - (Q_{0a}{}^2 V P_0 V)\} |\varphi> + \lambda^3 k^{-1} (..)|\varphi> + ...$$

We know that $k = (1 + \lambda^2 C + \lambda^3 E \cdots)$ so that $k^{-1} = 1 - \lambda^2 C + \lambda^3 D + ...$, so we get

$$|\psi> = |\varphi> + \lambda(1 - \lambda^2 C + \lambda^3 D + ..) Q_{0a} V|\varphi> +$$

$$+ \lambda^2 (1 - \lambda^2 C + \lambda^3 D + ..) \{ (Q_{0a} V Q_{0a} V) - (Q_{0a}{}^2 V P_0 V)\} |\varphi>$$

$$+ \lambda^3 (1 - \lambda^2 C + \lambda^3 D + ..) (..)|\varphi> + ...$$

and then we can collect powers of λ to get

$$|\psi> = |\varphi> + \lambda Q_{0a} V|\varphi> +$$

$$+ \lambda^2 \{ (Q_{0a} V Q_{0a} V) - (Q_{0a}{}^2 V P_0 V)\} |\varphi>$$

$$+ \lambda^3 \{ (..) - C Q_{0a} V \} |\varphi> + ...$$

where we show a λ^3 piece of the $Q_{0a} V|\varphi>$ term showing up now in the λ^3 term.

What we have learned here is that the Kato state expansion using $P^{(n)}$ and the M/S expansion are subtle *rearrangements* of each other, but that the λ^0, λ^1 and λ^2 terms of both expansions are the same, provided we drop the P_0-starting term in the λ^2 term. Thus we can now identify from the M/S expansion ,

$$|\psi> = |\varphi> + \Sigma_{n=1,\infty} \lambda^n |\psi ;n>$$

that we have

$$|\psi ;0> = |\varphi>$$

$$|\psi ;1> = \lambda Q_{0a} V|\varphi> \qquad \text{// agrees with Messiah p 680 (14)}$$

$$|\psi ;2> = \lambda^2 (Q_{0a} V Q_{0a} V - Q_{0a}{}^2 V P_0 V)|\varphi> \qquad \text{// agrees with Messiah p 694 (27)}$$

and we get agreement with the non-Kato method used earlier by Messiah.

We could of course use the Kato expansion "as is",

$$|\psi\rangle = \Sigma_{n=0}\, \lambda^n P^{(n)} |\varphi\rangle$$

if we are willing to have the normalization of $|\psi\rangle$ come out as it may (so no k^{-1}on the RHS), and if we are willing to have terms in the expansion which contain some $|\varphi\rangle$ component. We just have to keep in mind that this expansion of state corrections is then *different* from the fancy M/S expansion with its unusual requirements that $\langle\varphi\,|\psi\,;n\rangle = 0$. There is really something to be said in favor of the Kato expansion because it let's you see *all* the terms in each λ^n order that "appear", including terms proportional to $|\varphi\rangle$.

To summarize our Kato state correction method cast into the M/S convention

$$|\psi\rangle = |\varphi\rangle + k^{-1}\ \Sigma_{n=1}\, \lambda^n P'^{(n)} |\varphi\rangle$$

$$= |\varphi\rangle + \langle\varphi| \Sigma_{m=1}\, \lambda^m P^{(m)} |\varphi\rangle^{-1} \left[\ \Sigma_{k=1}\, \lambda^k\ P'^{(k)} |\varphi\rangle\ \right]$$

where $P'^{(n)}$ means we delete any terms that begin with P_0 in $P^{(n)}$. Thus we can say

$$|\psi\,;n\rangle\ =\ \text{coefficient of}\ \lambda^n\ \text{in}\ \left\{\ \langle\varphi| \Sigma_{m=1}\, \lambda^m P^{(m)} |\varphi\rangle^{-1} \left[\ \Sigma_{k=1}\, \lambda^k\ P'^{(k)} |\varphi\rangle\ \right]\ \right\}$$

Although this is well-defined, it is admittedly not very convenient (we did some examples above), and perhaps this is why Messiah did not mention this expansion method. Note that

$$(1+x)^{-1}\ = 1 - x + x^2 - x^3 + ...$$

so that

$$(1+ a\lambda^2 + b\lambda^3 + c\lambda^4)^{-1}\ =\ 1 -(a\lambda^2 + b\lambda^3 + c\lambda^4) + (a\lambda^2 + b\lambda^3 + c\lambda^4)^2 + ...$$

$$= 1 - a\lambda^2 - b\lambda^3 + (-c + a^2)\, \lambda^4\ + ...$$

so we could at least do it all if we had to.

Messiah on page 688 describes the *non-Kato* method of getting the state corrections. You use this iterative scheme:

$$|\psi\,;n\rangle\ = Q_{0a}(V-\varepsilon_1)\, |\psi\,;n-1\rangle\ - \varepsilon_2\, |\psi\,;n-2\rangle - ... - \varepsilon_{n-1}\, |\psi\,;1\rangle$$

and use this to get started: $|\psi\,;1\rangle\ = Q_{0a}V\, |\psi\,;0\rangle$ and $|\psi\,;0\rangle\ = |\varphi\rangle$

To use this iterative method, we need the ε_n. We can either get these from the method described below which says $\varepsilon_n = \text{tr}(B^{(n)}) = \langle\varphi| B'^{(n)} |\varphi\rangle$, or we could use the traditional double iteration method which is this:

$\|1\rangle\ = Q_{0a}V\, \|0\rangle$		1	s = 1
$\varepsilon_1 = \langle 0\| V\, \|0\rangle = V_{nn}$	**// Messiah p 689 (12)**	1	
$\|2\rangle\ = Q_{0a}V\, \|1\rangle\ - \varepsilon_1\, Q_{0a}\, \|1\rangle$		2	s = 2
$\varepsilon_2\ = \langle 0\| V\, \|1\rangle = \langle 0\|V\, Q_{0a}V\, \|0\rangle$	**// Messiah p 694 (26)**	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

where I show in the second last column the number of terms involved.

B. Comments of Messiah at the start of his $g_a = 1$ section page 717.

When I first read these comments, I had no idea what he was talking about, but now they all make sense.

$k|\psi\rangle = P|\varphi\rangle \quad \Rightarrow \quad k^2\langle\psi|\psi\rangle = \langle\varphi|P\,P|\varphi\rangle = \langle\varphi|P|\varphi\rangle$

"the norm (Messiah's norm) of $P|\varphi\rangle$ is $\| P|\varphi\rangle\|^2 = \langle\varphi|P|\varphi\rangle$ " agreed!

" insert P and you could compute $\langle\varphi|P|\varphi\rangle$" agreed!

" $P|\varphi\rangle$ is a multiple of the eigenvector $|\psi\rangle$ formed in Section I (that of the MS expansion) "

The above I would associate with my claim that $k|\psi\rangle = P|\varphi\rangle$. agreed!

"the norm (Messiah's norm)of the latter($|\psi\rangle$) is $1/\langle\varphi|P|\varphi\rangle$" agreed!

C. Computing the energy corrections

Our eigenvalue problem as noted above is this

$B''|\varphi\rangle = (E_\alpha - E_a^0)\,P''|\varphi\rangle$ // both sides are kets in $\mathcal{E}_a$

where $|\varphi\rangle$ is our unperturbed unit-normalized sole state in $\mathcal{E}_a^0$. We have already commented that $P|\varphi\rangle = k|\psi\rangle$ where $k = \langle\varphi|P|\varphi\rangle$. Our expansion above became

$$k|\psi\rangle = k|\varphi\rangle + \lambda Q_{0a}V|\varphi\rangle$$

$$+ \lambda^2 \{ (Q_{0a}VQ_{0a}V) - (Q_{0a}^2VP_0V) \}|\varphi\rangle + \lambda^3 (..)|\varphi\rangle + ...$$

where no terms on the RHS other than the first have any component in $|\varphi\rangle$. Therefore, we may conclude that $P_0|\psi\rangle = |\varphi\rangle$. Of course to make this work, we have to delete any terms on the RHS that begin with P_0. Assume we do this. Then we have for our two projectors:

$P_0|\psi\rangle = |\varphi\rangle$ and $P|\varphi\rangle = k|\psi\rangle$

$P_0|\varphi\rangle = |\varphi\rangle$ and $P|\psi\rangle = |\psi\rangle$

$k = \langle\varphi| P |\varphi\rangle = 1 + \langle\varphi| \Sigma_{n=1} \lambda^n P^{(n)}|\varphi\rangle = (1 + \lambda^2 C + \lambda^3 C' + \lambda^4 C'' + ...)$

The first line shows our 1-to-1 pair of mappings in the case each space has only one state! The ket $|\varphi\rangle$ is normalized to unity, but $|\psi\rangle$ is not so normalized. In fact, we know $\langle\psi|\psi\rangle = 1/k$.

Our equation above says

$P_0BP_0|\varphi\rangle = (E_\alpha - E_a^0) P_0PP_0|\varphi\rangle$

But look at the RHS operator

$P_0PP_0|\varphi\rangle = P_0P|\varphi\rangle = k P_0 |\psi\rangle = k |\varphi\rangle$

so we end up with

$P_0BP_0|\varphi\rangle = k (E_\alpha - E_a^0) |\varphi\rangle$ // all terms in B are included here, φ is normalized

and thus, since $\langle\varphi|\varphi\rangle = 1$,

$k (E_\alpha - E_a^0) = \langle\varphi|B|\varphi\rangle = \Sigma_{n=1} \lambda^n \langle\varphi| B^{(n)}|\varphi\rangle$

Thus we get

$E_\alpha = E_a^0 + k^{-1} \Sigma_{n=1} \lambda^n \langle\varphi| B^{(n)}|\varphi\rangle = E_a^0 + k^{-1} \Sigma_{n=1} \lambda^n \langle\varphi| B^{(n)}|\varphi\rangle$

$= E_a^0 + (1 - \lambda^2 C + \lambda^3 D + ..) \Sigma_{n=1} \lambda^n \langle\varphi| B^{(n)}|\varphi\rangle$

$= E_a^0 + (1 - \lambda^2 C + \lambda^3 D + ..) (\lambda\langle\varphi| B^{(1)}|\varphi\rangle + \lambda^2\langle\varphi| B^{(2)}|\varphi\rangle + ...)$

$= E_a^0 + \lambda\langle\varphi| B^{(1)}|\varphi\rangle + \lambda^2\langle\varphi| B^{(2)}|\varphi\rangle + \lambda^3\{ \langle\varphi| B^{(3)}|\varphi\rangle - C\langle\varphi| B^{(1)}|\varphi\rangle \} + ...$

Notice this correction we get on the λ^3 term, we come back to this below. In theory, we could compute our constant $k = \langle\varphi|P|\varphi\rangle$ to any desired order, and then we could write out the above energy corrections to any order. It turns out that there is an easier way to do this, but we hold off on that for a moment and continue along here to show that things really work right.

To compute the first two terms above, we look up

$B^{(1)} = P_0VP_0 \approx V$

$B^{(2)} = (Q_{0a}VP_0VP_0 + 2 \text{ perms}) \approx P_0VQ_{0a}VP_0 \approx VQ_{0a}V$

In order to compute the λ^3 term, we look up the following facts:

$C = -\langle\varphi| VQ_{0a}^2V|\varphi\rangle$

$B^{(3)} = -(Q_{0a}^2VP_0VP_0VP_0 + 3 \text{ perms}) + (Q_{0a}VQ_{0a}V\,P_0VP_0 + 5 \text{ perms})$

$\approx -(P_0VQ_{0a}^2VP_0VP_0 + P_0V\,P_0\,VQ_{0a}^2VP_0) + P_0VQ_{0a}VQ_{0a}V\,P_0$

$\approx VQ_{0a}VQ_{0a}V - (VQ_{0a}^2VP_0V + V\,P_0\,VQ_{0a}^2V)$

$B^{(1)} = P_0VP_0 \approx V$

Thus, the λ^3 term is given by

$\lambda^3\{\langle\varphi| B^{(3)}|\varphi\rangle - C\langle\varphi| B^{(1)}|\varphi\rangle\}$

$= \lambda^3\langle\varphi|\{B^{(3)} - C\,B^{(1)}\}|\varphi\rangle$

$= \lambda^3\langle\varphi|\{VQ_{0a}VQ_{0a}V - (VQ_{0a}^2VP_0V + V\,P_0\,VQ_{0a}^2V) + \langle\varphi| VQ_{0a}^2V|\varphi\rangle V\}|\varphi\rangle$

The last term can be written:

$\lambda^3\langle\varphi|\langle\varphi| VQ_{0a}^2V|\varphi\rangle V\}|\varphi\rangle = \lambda^3\langle\varphi| V|\varphi\rangle\langle\varphi| VQ_{0a}^2V|\varphi\rangle = \lambda^3\langle\varphi| VP_0VQ_{0a}^2V|\varphi\rangle$

so that the sum is now

$= \lambda^3\langle\varphi|\{VQ_{0a}VQ_{0a}V - (VQ_{0a}^2VP_0V + V\,P_0VQ_{0a}^2V) + VP_0VQ_{0a}^2V\}|\varphi\rangle$

$= \lambda^3\langle\varphi|\{VQ_{0a}VQ_{0a}V - VQ_{0a}^2VP_0V\}|\varphi\rangle$

since the last two terms cancel.

So we may now summarize the first three energy correction terms:

$E_\alpha = E_a^0 + \lambda\langle\varphi| B^{(1)}|\varphi\rangle + \lambda^2\langle\varphi| B^{(2)}|\varphi\rangle + \lambda^3\{\langle\varphi| B^{(3)}|\varphi\rangle - C\langle\varphi| B^{(1)}|\varphi\rangle\} + \ldots$

$= E_a^0 + \lambda\langle\varphi| V|\varphi\rangle + \lambda^2\langle\varphi| VQ_{0a}V|\varphi\rangle + \lambda^3\langle\varphi|\{VQ_{0a}VQ_{0a}V - VQ_{0a}^2VP_0V\}|\varphi\rangle$

and this agrees exactly with Messiah page 717 (74), although he used a different method to arrive at this result. We can compare his method and our method for finding the eigenenergies:

Our method here:

$k(E_\alpha - E_a^0) = \langle\varphi|B|\varphi\rangle = \Sigma_{n=1}\,\lambda^n\langle\varphi| B^{(n)}|\varphi\rangle \quad \Rightarrow$

$\varepsilon_n = \langle\varphi| B^{(n)}|\varphi\rangle = \langle\varphi| B^{(n)}|\varphi\rangle / \langle\varphi|P|\varphi\rangle$

Messiah's method used earlier was this (see Round Three notes p ~ 15),

$$\varepsilon_n = \mathrm{tr}(B^{(n)}) = \langle\varphi| B'^{(n)} |\varphi\rangle$$

where prime means we knock out any one P_0 factor in each subterm of $B^{(n)}$. This is a more direct way to compute the energy corrections to arbitrary order. A clean and simple prescription.

Comparing our methods, the following interesting fact must be true

$$\langle\varphi| B^{(n)} |\varphi\rangle = \langle\varphi| B'^{(n)} |\varphi\rangle \langle\varphi|P|\varphi\rangle = \langle\varphi| B'^{(n)} P_0 P |\varphi\rangle \qquad \text{// definition of } P_0$$

I tried proving this going back and forth between the trace and $\langle\varphi|...|\varphi\rangle$ forms, but that does not seem to do the trick! This is some kind of more global theorem. See appendix A below for more comments.

Appendix A

Another approach is to write out the explicit form of $B^{(n)}$

$$B^{(n)} = \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] \qquad \text{// sum on all indices that sum to n-1}$$

$$P^{(n)} = \Sigma_{(n)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$$

where $R_0 \equiv P_0$ and $R_k \equiv (-1)^{k-1} (Q_{0a})^k$ $k>0$

Then the theorem must state that

$$\langle\varphi| \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] |\varphi\rangle$$

$$= \langle\varphi| \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}], \text{ one } P_0 \text{ knocked out } |\varphi\rangle$$
$$* \langle\varphi| \Sigma_n \lambda^n \Sigma_{(n)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] |\varphi\rangle$$

$$= \Sigma_n \lambda^n \langle\varphi| \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}], \text{ one } P_0 \text{ knocked out } * P_0 \Sigma_{(n)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] |\varphi\rangle$$

I have to say this theorem is very non-obvious when viewed in this manner! But in fact we have already proven it, so I will formally declare a theorem

Theorem: $\langle\varphi| B^{(n)} |\varphi\rangle = \langle\varphi| B'^{(n)} |\varphi\rangle \langle\varphi|P|\varphi\rangle = \langle\varphi| B'^{(n)} P_0 P |\varphi\rangle$

Proof: We compute ε_n (our energy correction in n^{th} order) by two different valid methods, and comparing the results proves the theorem. It looks like renormalization.

One more try: the above also says

$\langle\varphi| \Sigma_{(n-1)}[R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] |\varphi\rangle$

$= \langle\varphi| \Sigma_n \lambda^n \Sigma_{(n)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] |\varphi\rangle$

$* \langle\varphi| \Sigma_{(n-1)}[R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$, one P_0 knocked out $|\varphi\rangle$

$= \Sigma_n \lambda^n \Sigma_{(n,i)} \langle\varphi| [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] P_0$
$\Sigma_{(n-1,j)}[R_{j_0} V R_{j_1} V \ldots\ldots V R_{j_n}]$, one P_0 knocked out $|\varphi\rangle$

$= \Sigma_n \lambda^n \Sigma_{(n,i)} \Sigma_{(n-1,j)}$

$\langle\varphi| [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] P_0 [R_{j_0} V R_{j_1} V \ldots\ldots V R_{j_n}]_{\text{one P0 knocked out}} |\varphi\rangle$

This is a combinatoric problem which I don't know how to solve. Let's call it quits in this!