Kato Round Three PhL 2.2.09

I intended this round to be my final meta notes, and started off in a very organized manner. But then I ended up getting way down into details, so this then became Round Three and meta notes were put off to the next and last document.

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Section 15 and Section 16

Definition of G(z)

1. A bound state problem has some Hamiltonian H, and the **resolvent** is defined simply as

$$G(z) = (z-H)^{-1} \qquad (1)$$

an operator function of complex variable z.

Definition of $\psi_{i,n}$ and E_i and P_i

2. The problem has a state and energy spectrum which can be decomposed into a direct sum of subspace problems in the usual manner. For subspace S_i we have eigenvectors $\{\psi_{i,n}\}$ such that

$$H\psi_{i,n} = E_i\psi_{i,n} \qquad\qquad HP_i = E_iP_i \qquad\qquad (2)$$

where P_i is the usual **projector** for S_i. The equation on the right may be verified by applying it to all states in the Hilbert Space (HS) of the entire problem. For states not in S_i it says 0 = 0. Otherwise, it repeats the left equation. We know that $\Sigma_i P_i = 1$ if we add up over all subspaces of the problem. Any subspace S_i could be non-degenerate (dimension = 1) or could be degenerate (dimension > 1).

The projector-pole expansion of G(z)

3. Applying (2) to (1) we find that

$$G(z)\,P_i = (z-H)^{-1}P_i = (z-E_i)^{-1}P_i \qquad => \qquad G(z) = \Sigma_i\,(z-E_i)^{-1}P_i \qquad (3)$$

where we just applied Σ_i over subspaces to both sides of the first equation to get (3).

Projector P_i is the residue of the pole of G(z) at z-E_i

4. Now apply a contour integral to both sides of (3) and use the usual residue formula for a simple pole to get

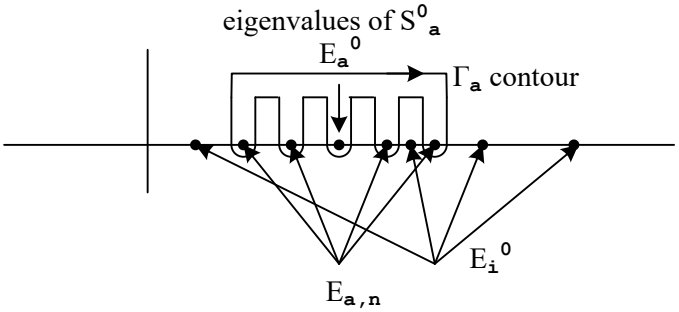
$$P_i = (2\pi i)^{-1} \int_{\Gamma i} dz\, G(z) \qquad (4)$$

where the contour Γ_i captures the pole at $z = E_i$. We could imagine another contour which captures some *set* of poles $\{E_i\}$, thus making a projector which projects onto the subspace spanned by the corresponding set of states $\{\psi_i\}$. We will be doing that next.

Definition of $\psi_{a,n}$ and $E_{a,n}$; of $\varphi_{a,i}$ and E_a^0 ; and of N and $\mathcal{E}_a$ and $\mathcal{E}_a^0$ and Γ_a

5. Now assume $H = H_0 + \lambda V$ and we are doing perturbation theory. When the perturbation is turned on, imagine that the equation $H\psi = E\psi$ has a certain set of N eigenvectors $\psi_{a,n}$ with eigenenergies $E_{a,n}$ *which*, when the perturbation is gradually turned off ($\lambda \to 0$), become N degenerate eigenvectors $\varphi_{a,n}$ of H_0, all having the same eigenenergy E_a^0. This is the key concept. We then want to define two distinct N dimensional spaces: space $\mathcal{E}_a$ is that spanned by the set of $\psi_{a,n}$ just mentioned, while $\mathcal{E}_a^0$ is that spanned by the degenerate $\varphi_{a,n}$. As $\lambda \to 0$. we can certainly claim that $\mathcal{E}_a \to \mathcal{E}_a^0$. Clearly $\mathcal{E}_a^0$ is a subspace of the H_0 problem. The space $\mathcal{E}_a$ is the union of at most N subspaces S_i of the H problem: the number would be N only if it happened that all the $\psi_{a,n}$ were non-degenerate. It does not matter to us whether any of the subspaces whose union is $\mathcal{E}_a$ is degenerate.

Now imagine we create a contour Γ_a in the z plane which is carefully designed to circulate (in the usual sense) all the locations $z = \{E_{a,n}\}$ as well as the location $z = E_a^0$. This contour is also selected so as to *not* include in its circulation any z locations associated with the eigenenergies of other subspaces $\mathcal{E}_i^0$ or $\mathcal{E}_i$ where $i \neq a$. In the following picture, I show a few eigenenergies of some $\mathcal{E}_i^0$ $i \neq a$ that lie outside the contour:



So clearly we can think of the Γ_a contour as equivalent to a sum of N Γ_n contours around pole locations $z = \{E_{a,n}\}$ of the operator function G(z). Each of these contours yields a P_n for that pole residue, and the sum of the P_n we shall call P. P then is the projection operator which projects out of any ket that portion lying in space $\mathcal{E}_a$:

$$P = \Sigma_{n=1}^{N} P_n = \Sigma_{n=1}^{N} \{ (2\pi i)^{-1} \int_{\Gamma n} dz\, G(z) \} = (2\pi i)^{-1} \int_{\Gamma a} dz\, G(z)$$

The Kato formulas for P and HP

6. Since $G(z) \equiv (z-H)^{-1}$, we know that $(z-H)G = 1$ which says $zG = 1+HG$. Therefore

$$(2\pi i)^{-1} \int_{\Gamma a} dz\, zG(z) = (2\pi i)^{-1} \int_{\Gamma a} dz\, [1+HG(z)] = (2\pi i)^{-1} H \int_{\Gamma a} dz\, G(z) = HP.$$

since the contour integral of 1 is 0, and H is not a function of z, and using (4) above for P. So let us restate this and the previous result, which are the main weapons in the Kato arsenal:

$$P = (2\pi i)^{-1} \int_{\Gamma a} dz\, G(z) \qquad (5a)$$

$$HP = (2\pi i)^{-1} \int_{\Gamma a} dz\, z\, G(z) \qquad (5b)$$

The expressions are identical apart from an extra factor of z in the HP integrand.

Integral equation for G(z) and its series solution which is then installed into the Kato formulas

7. We can define both $G(z) \equiv (z-H)^{-1}$ and $G_0(z) \equiv (z-H_0)^{-1}$ where $H = H_0 + \lambda V$. Very simple algebra then shows that

$$G = G_o(1 + \lambda VG) \qquad (6)$$

which is an operator equation for G. Our perturbation problem presumably concerns the motion of a single particle under Hamiltonian H. Were we to work in the coordinate space representation, for example, and were we to define $G(r,r') \equiv \langle r|G|r'\rangle$ and similarly for G_o and V, we would write (6) as

$$G(r,r') = G_0(r,r') + \lambda \int d^3r'' \; V(r,r'')G(r'',r')$$

and we would refer to this as "an integral equation for G". The equation certainly resembles integral equations we commonly see in scattering theory, but here we are dealing with a bound state problem.

8. Just as we do in scattering theory, we can derive a series solution of (6) which has this form:

$$G = \Sigma_{n=0}^{\infty} \lambda^n G_0(VG_0)^n = G_0 + \lambda G_0VG_0 + \lambda^2 G_0VG_0VG_0 + ... \qquad (7)$$

In any event, it is trivial to show that the series (7) solves our operator equation (6):

$$RHS = G_o(1 + \lambda VG) = G_o(1 + \lambda V \Sigma_{n=0}^{\infty} \lambda^n G_0(VG_0)^n) = G_o + \lambda \Sigma_{n=0}^{\infty} \lambda^n G_oVG_0(VG_0)^n$$

$$= G_o + \Sigma_{n=0}^{\infty} \lambda^{n+1} G_o(VG_0)^{n+1} = G_o + \Sigma_{m=1}^{\infty} \lambda^m G_o(VG_0)^m = \Sigma_{m=0}^{\infty} \lambda^m G_o(VG_0)^m = LHS$$

9. We now use for G(z) in (4) and (5) our series solution (7) to get these new Kato formulas:

$$P = (2\pi i)^{-1} \int_{\Gamma a} dz \; G(z) \quad = \Sigma_{n=0}^{\infty} \lambda^n \; (2\pi i)^{-1} \int_{\Gamma a} dz \; G_0(VG_0)^n \qquad (8)$$

$$HP = (2\pi i)^{-1} \int_{\Gamma a} dz \; zG(z) \; = \Sigma_{n=0}^{\infty} \lambda^n \; (2\pi i)^{-1} \int_{\Gamma a} dz \; z \; G_0(VG_0)^n \qquad (9)$$

We are now going to interpret (8) and (9) as expansions in smallness parameter λ for our two operators P and HP. As noted earlier, P projects things onto space $\mathcal{E}_a$, while H is the full Hamiltonian including the perturbing term. So the above pair of equations become

$$P = \Sigma_{n=0}^{\infty} \lambda^n \; P^{(n)} \qquad P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz \; G_0(VG_0)^n \qquad (8')$$

$$HP = \Sigma_{n=0}^{\infty} \lambda^n \; (HP)^{(n)} \qquad (HP)^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz \; z \; G_0(VG_0)^n \qquad (9')$$

We want to evaluate these contour integrals which means we need to learn about the z-plane structure of G_0, which we now ponder.

The projector-pole expansion of $G_0(z)$: definition of P_i^0 and $P_0 \equiv P_a^0$

10. We are now going to repeat the work of sections 1,2,3 above, but for $G_0(z)$ instead of G(z). The first two sections yield these equations

$$G_0(z) \equiv (z-H_0)^{-1} \qquad (1)_0$$

$$H_0\varphi_{i,n} = E_i{}^0\varphi_{i,n} \qquad H_0P_i{}^0 = E_i{}^0P_i{}^0 \qquad (2)_0$$

where the φ_i span the (possibly degenerate) subspace of eigenvalue $E_i{}^0$, and where $P_i{}^0$ projects out of any ket that portion which lies in the subspace $S_i{}^0$ spanned by the φ_i. We apologize for the fact that some of the 0's are subscripts while others are superscripts. For equation 3 then we have

$$G_0(z)\, P_i{}^0 = (z-H_0)^{-1}P_i{}^0 = (z-E_i{}^0)^{-1}P_i{}^0 \qquad =>$$

$$G_0(z) = \Sigma_i\, (z-E_i{}^0)^{-1}P_i{}^0 \qquad (3)_0$$

where Σ_i is over all the subspaces of operator H_0. One of the subspaces in this sum is $\mathcal{E}_a{}^0$ above, having projector $P_a{}^0 \equiv P_0$. We can break out this one subspace and say

$$G_0(z) = (z-E_a{}^0)^{-1}P_0 + \Sigma_{i\neq a}\, (z-E_i{}^0)^{-1}P_i{}^0 \qquad (10)$$

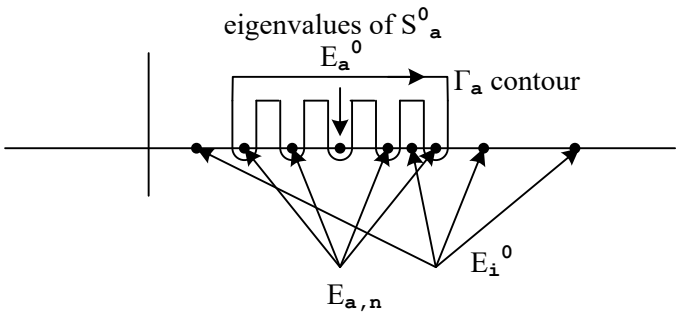
where the remaining sum is over *other* subspaces of H_0.

Examination of a sample Kato integral

11. Were we to simply install this expression for $G_0(z)$ into the Kato series expansions (8) and (9) above, we would have terms of this general form (we use the simple n=1 term of (8) as an example)

$$\int_{\Gamma a} dz\, G_0VG_0 = \int_{\Gamma a} dz\, \{(z-E_a{}^0)^{-1}P_0 + \Sigma_{i\neq a}\, (z-E_i{}^0)^{-1}\, P_i{}^0\, \}$$
$$V\{(z-E_a{}^0)^{-1}P_0 + \Sigma_{i'\neq a}\, (z-E_{i'}{}^0)^{-1}P_{i'}{}^0\}$$

The contour Γ_a was selected to include the $E_{a,n}$ eigenenergies as well as the eigenenergy $E_a{}^0$. The eigenenergies $E_{a,n}$ were some of the poles of G(z). Now that we have done a *series expansion* for G(z), we see that the expansion terms like the one shown above do not have poles at $E_{a,n}$. Instead, a particular term has a pole at $E_a{}^0$ and also has poles at other $E_i{}^0$ which lie outside our contour:



Therefore we may deform our contour to become a simple circulation about the pole at $z = E_a^0$.

The integrand has four terms. The first has a double pole at $z = E_a^0$ and integrates to 0. The fourth term has poles which all lie outside our contour and so also do not contribute. We are left then with the two cross terms, the first of which is this:

$$(2\pi i)^{-1} \int_{\Gamma a} dz \; \{(z-E_a^0)^{-1} P_0\} V \{\Sigma_{i \neq a} (z-E_i^0)^{-1} P_i^0\} \; = \; \Sigma_{i \neq a} \; P_0 \, V \, (E_a^0 - E_i^0)^{-1} P_i^0$$

where we have written out the residue of the pole at $z = E_a^0$. Below we will show this fact

$$[\, \Sigma_{i \neq a} \, (E_a^0 - E_i^0)^{-1} \, P_i^0] \; = Q_{0a}$$

which allows this term to be written as simply $P_0 V Q_{0a}$ and the other term is $Q_{0a} V P_0$. This shows the general idea, but we want to follow Kato's systematic presentation of this idea.

Kato's Bag of Tricks

A Taylor Series Expansion

12. Suppose some function f(z) is analytic at z=a. We can expand f(z) in the following Taylor series around the point z = a as follows:

$$f(z) = f(a) + \Sigma_{n=1,\infty} \, [\, f^{(n)}(a)/\, n! \,] \, (z-a)^n$$

Let's apply this to f(z) = (z-a)/(z-b). A quick calculation shows that

$$f^{(0)}(z) = (z-a)/(z-b) \qquad n=0$$
$$f^{(n)}(z) \; = (a-b) \, (-1)^{n-1} \, n! \, (z-b)^{-(n+1)} \qquad n>0$$

so that

$$f(a) = (a-a)/(a-b) \; = \; 0 \qquad n=0$$
$$f^{(n)}(a) \; = (-1)^{n-1} \, n! \, (a-b)^{-n} \qquad n>0$$

So we then have derived this Taylor expansion

$$(z\text{-}a)/(z\text{-}b) \;=\; \Sigma_{n=1,\infty}\,[(-1)^{n-1}\;(a\text{-}b)^{-n}\;]\,(z\text{-}a)^{n}$$

[The LHS has a pole at z=b. The RHS equals $-\Sigma_{n=1,\infty}\,1$ at this point and thus diverges. The LHS has a zero at z=a and the RHS is also zero at this point. This series probably converges in any disk around z=a with radius less than |b-a|.]

Now let's apply our Taylor expansion above setting $a = E_a^0$ and $b = E_i^0$:

$$(z\text{-}E_a^0)/(z\text{-}E_i^0) \;=\; \Sigma_{n=1,\infty}\,[(-1)^{n-1}\;(E_a^0\text{-}E_i^0)^{-n}\;]\,(z\text{-}E_a^0)^{n} \qquad (11)$$

Use this expansion in our formula for $G_0(z)$

13. Recall now our expansion above for $G_0(z)$, equation (10) above

$$G_0(z) = (z\text{-}E_a^0)^{-1}P_0 \;+\Sigma_{i\neq a}\,(z\text{-}E_i^0)^{-1}P_i^0 \;\;=\; (z\text{-}E_a^0)^{-1}P_0 \;+X$$

The second term which we shall call X has poles at all the locations $z = E_i^0$ (which lie outside our contour). Now let's process this second term X,

$$X = \Sigma_{i\neq a}\,(z\text{-}E_i^0)^{-1}P_i^0 \;=\; (z\text{-}E_a^0)^{-1}\,\Sigma_{i\neq a}\,\{(z\text{-}E_a^0)/(z\text{-}E_i^0)\}\;P_i^0$$

Then with the Taylor expansion (11) above, X becomes

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

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

where $\Sigma_{i\neq a}$ sums over all the subspaces of H_0 other than $\mathcal{E}_a^0$. So

$$G_0(z) = \;P_0/\,(z\text{-}E_a^0) + \Sigma_{n=1,\infty}\,(-1)^{n-1}\,(z\text{-}E_a^0)^{n-1}\,[\,\Sigma_{i\neq a}\,(E_a^0\text{-}E_i^0)^{-n}\,P_i^0] \qquad (12)$$

We are now going to come up with a compact way to express the last factor [...].

But first just a comment. Compare the above with our previous expression for $G_0(z)$,

$$G_0(z) = \;(z\text{-}E_a^0)^{-1}P_0 \;+\Sigma_{i\neq a}\,(z\text{-}E_i^0)^{-1}P_i^0$$

The operator function $G_0(z)$ really does have poles at the points $z = E_i^0$ as this last expression shows. The series expansion we used to get the previous expression for G_0 is not valid near these poles, and that is why we don't see any poles at $z = E_i^0$ in that expression! But we don't intend to use this second expression near those poles, so it is OK. We only use this second expression near the point $z = E_a^0$ since that is where our contracted contour lies.

Rewriting the $G_0(z)$ in terms of the operator Q_{0a}

14. We know that

$$1 = \Sigma_i P_i^0 = P_a^0 + \Sigma_{i\neq a} P_i^0 = P_0 + \Sigma_{i\neq a} P_i^0$$

where we are summing over subspaces of H_0. Suppose the eigenstates of subspace S_i^0 are called $\varphi_{i,n}$. Then we can write,

$$P_i^0 = \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \tag{13}$$

where n_i enumerates however many eigenstates span the subspace S_i^0.

Let's now define two new operators as follows

$$Q_0 \equiv 1 - P_0 = \Sigma_{i\neq a} P_i^0 = \Sigma_{i\neq a} \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \tag{14}$$

$$Q_{0a} \equiv Q_0 (E_a^0 - H_0)^{-1} Q_0 \tag{15}$$

The state sum appearing in Q_0 includes all eigenstates of H_0 *except* those in $\mathcal{E}_a^0$. So one can say that the operator Q_0 projects out of any ket the part that is in the perp space $(\mathcal{E}_a^0)^{\perp}$. Note that $Q_0^2 = Q_0$ which is true for *any* projection operator. We now claim this little theorem for the Q_{0a} operator

$$(Q_{0a})^n = Q_0 (E_a^0 - H_0)^{-n} Q_0 \tag{16}$$

and demonstrate it for the case n=2, where we use $H_0 |\varphi_{i,ni}\rangle = E_i^0 |\varphi_{i,ni}\rangle$ in both directions,

$$(Q_{0a})^2 = Q_0 (E_a^0 - H_0)^{-1} Q_0 \, Q_0 (E_a^0 - H_0)^{-1} Q_0 =$$

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

$$= Q_0 (E_a^0 - H_0)^{-1} \Sigma_{i\neq a} \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \quad (E_a^0 - H_0)^{-1} Q_0$$

$$= Q_0 (E_a^0 - E_i^0)^{-1} \Sigma_{i\neq a} \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \, (E_a^0 - E_i^0)^{-1} Q_0$$

$$= Q_0 (E_a^0 - E_i^0)^{-2} \Sigma_{i\neq a} \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \, Q_0$$

$$= Q_0 (E_a^0 - H_0)^{-2} \Sigma_{i\neq a} \Sigma_{ni} \, |\varphi_{i,ni}\rangle\langle\varphi_{i,ni}| \, Q_0$$

$$= Q_0 (E_a^0 - H_0)^{-2} Q_0 \, Q_0 = Q_0 (E_a^0 - H_0)^{-2} Q_0 \qquad \text{QED}$$

We are now going to show that our factor [...] in (12) is given by

$$[\, \Sigma_{i\neq a} (E_a^0 - E_i^0)^{-n} P_i^0] = (Q_{0a})^n \tag{17}$$

We start with the RHS and use our theorem above

$$(Q_{0a})^n = Q_0 (E_a^0 - H_0)^{-n} Q_0 = \Sigma_{i\neq a} \Sigma_{ni} | \varphi_{i,ni}\rangle\langle \varphi_{i,ni}| (E_a^0 - H_0)^{-n} Q_0$$

$$= \Sigma_{i\neq a} \Sigma_{ni} | \varphi_{i,ni}\rangle\langle \varphi_{i,ni}| (E_a^0 - E_i^0)^{-n} Q_0$$

$$= \Sigma_{i\neq a} \Sigma_{ni} | \varphi_{i,ni}\rangle\langle \varphi_{i,ni}| (E_a^0 - E_i^0)^{-n} \Sigma_{j\neq a} \Sigma_{nj} | \varphi_{j,nj}\rangle\langle \varphi_{j,nj}|$$

$$= \Sigma_{i\neq a} \Sigma_{ni} \Sigma_{j\neq a} \Sigma_{nj} (E_a^0 - E_i^0)^{-n} \langle \varphi_{i,ni}| \varphi_{j,nj}\rangle | \varphi_{i,ni}\rangle\langle \varphi_{j,nj}|$$

$$= \Sigma_{i\neq a} \Sigma_{ni} \Sigma_{j\neq a} \Sigma_{nj} (E_a^0 - E_i^0)^{-n} \delta_{i,j} \delta_{ni,nj} | \varphi_{i,ni}\rangle\langle \varphi_{j,nj}|$$

$$= \Sigma_{i\neq a} \Sigma_{ni} (E_a^0 - E_i^0)^{-n} | \varphi_{i,ni}\rangle\langle \varphi_{i,ni}|$$

$$= \Sigma_{i\neq a} (E_a^0 - E_i^0)^{-n} \Sigma_{ni} | \varphi_{i,ni}\rangle\langle \varphi_{i,ni}|$$

$$= \Sigma_{i\neq a} (E_a^0 - E_i^0)^{-n} P_i^0$$

where we have assumed that eigenfunctions are orthonormalized in each subspace S_i^0. We have now shown this fairly impressive and compact operator expansion for $G_0(z)$

$$G_0(z) = P_0/ (z-E_a^0) + \Sigma_{n=1,\infty} (-1)^{n-1} (z - E_a^0)^{n-1} (Q_{0a})^n \qquad (18)$$

Notice that all the z-dependence is of the form $(z-E_a^0)$. The first term has a pole at $z = E_a^0$. The series part is analytic at $z = E_a^0$ and the nth term in the series has a zero of degree n-1 at $z = E_a^0$. It is now helpful to make (18) even more compact as follows:

$$G_0(z) = \Sigma_{n=0,\infty} R_n y^{n-1} \qquad (19)$$

where

$$y \equiv (z-E_a^0) \qquad R_0 \equiv P_0 \qquad \text{and } R_n \equiv (-1)^{n-1} (Q_{0a})^n \qquad \text{for } n>0$$

so

$$R_1 = Q_{0a} \qquad R_2 = - Q_{0a}^2 \qquad R_3 = Q_{0a}^3 \qquad \text{etc}$$

Notice that, in each term in the sum for $G_0(z)$, the index of the coefficient operator R_n is one larger than the exponent of the matching power of y. Normally we are used to seeing these numbers be the same in a series. This fact leads to the following mini-theorem.

A mini-theorem about powers of $G_0(z)$

15. Consider this operator

$$F \equiv [G_0(z)]^{n+1} = [\Sigma_{i=0,\infty} R_i y^{i-1}]^{n+1}$$

$$= \{ \Sigma_{i_0=0,\infty} R_{i_0} y^{i_0-1} \} \{ \Sigma_{i_1=0,\infty} R_{i_1} y^{i_1-1} \} .. \{ \Sigma_{i_n=0,\infty} R_{i_n} y^{i_n-1} \}$$

where we have n+1 summation indices i_0 through i_n .

Theorem: If the exponents of y of a particular term in this (n+1)-fold product add up to J, then the sum of the indices on the corresponding R_i for that same term add up to J + (n+1).

The proof is that there are (n+1) factors in a particular term, and for each such factor the index of R is one more than the exponent of y, so the sum of the exponents must exceed the sum of the indices of R by n+1.

Corollary: Suppose the exponents of y add up to -1. Then the indices of R add up to -1 + (n+1) = n.

Generalization: Both the theorem and corollary would be valid for an operator of the more general form

$$F' \equiv G_0(z) A_1 G_0(z) A_2 .....A_n G_0(z)$$

where there are n operators A_i sandwiched between pairs of G_0 factors. If we set all the $A_i = V$, then this is exactly the situation that arises in the Kato integrals, as we shall see.

Evaluation of a demonstration Kato integral

16. Now let's look what happens when we use this expansion (18) to evaluate a sample Kato integral. We consider the same case we considered back in section (11),

$$\int_{\Gamma a} dz\, G_0 V G_0 = \int_{\Gamma a} dz \{ P_0/(z-E_a^0) + \Sigma_{n=1,\infty} (-1)^{n+1} (z-E_a^0)^{n-1} (Q_{0a})^n \}$$
$$V \{ P_0/(z-E_a^0) + \Sigma_{m=1,\infty} (-1)^{m+1} (z-E_a^0)^{m-1} (Q_{0a})^m \}$$

$$= \oint_{y=0} dy \{ \Sigma_{n=0,\infty} R_n y^{n-1} \} V \{ \Sigma_{m=0,\infty} R_m y^{m-1} \} \qquad // \; y \equiv (z-E_a^0)$$

where now the contour encircles y = 0 instead of z = E_a^0. Let's write out a few terms:

$$= \oint_{y=0} dy \{ R_0 y^{-1} + R_1 + R_2 y + R_3 y^3 + ... \} V \{ R_0 y^{-1} + R_1 + R_2 y + R_3 y^3 + ... \}$$

If we think of this integral in terms of our mini-theorem above, there are n+1 = 2 factors of G_0 involved, so n = 1. Our corollary tells us that any term which has a sum of y exponents adding up to -1 will have R indices adding up to -1 + (n+1) = +1. Of course it is only terms whose y exponents add up to -1 which contribute to the contour integral because only these terms are simple poles. All other terms in the integrand result in double poles, constants, or zeros, all of which yield 0.

Using this rule (or just staring at the example above), one may evaluate the integral "by inspection":

$$\int_{\Gamma a} dz\, G_0 V G_0 = (2\pi i)(R_0 V R_1 + R_1 V R_0) = (2\pi i)(P_0 V Q_{0a} + Q_{0a} V P_0)$$

Evaluation of all the Kato integrals

17. We now return to (8) and (9) above which we copy here

$$P = (2\pi i)^{-1} \int_{\Gamma a} dz\, G(z) \quad = \Sigma_{n=0}^{\infty} \lambda^n \; (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n \qquad (8)$$

$$HP = (2\pi i)^{-1} \int_{\Gamma a} dz\, zG(z) \; = \Sigma_{n=0}^{\infty} \lambda^n \; (2\pi i)^{-1} \int_{\Gamma a} dz\, z\, G_0(VG_0)^n \qquad (9)$$

We are now going to interpret (8) and (9) as expansions in smallness parameter λ for our two operators P and HP. As noted earlier, P projects out of kets the portion lying in space $\mathcal{E}_a$, while H is the full Hamiltonian $H = H_0 + \lambda V$. The reason we want to do these expansions will be revealed later. So the above pair of equations become

$$P = \Sigma_{n=0}^{\infty} \lambda^n \; P^{(n)} \qquad\qquad P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n$$

$$HP = \Sigma_{n=0}^{\infty} \lambda^n \; (HP)^{(n)} \qquad\qquad (HP)^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, z\, G_0(VG_0)^n$$

We don't have any wonderful interpretation for operators like $P^{(n)}$ or $(HP)^{(n)}$ other than they are the λ^n component of P and HP expanded as shown.

We start with the simpler $P^{(n)}$ integral.

$$P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n \;\; = \;\; (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0 V\, G_0 V \ldots\ldots V G_0$$

There are n factors of V (which is why this term is order λ^n), and n+1 factors of $G_0(z)$. If we convert from dz to dy as in our sample integral, this becomes, using (19) $G_0(z) = \Sigma_{i=1,\infty} R_i\, y^{i-1}$,

$$= \; (2\pi i)^{-1} \int_{\Gamma a} dy \; \{ \Sigma_{i_0=0,\infty} R_{i_0}\, y^{i_0-1} \} V \; \{ \Sigma_{i_1=0,\infty} R_{i_1}\, y^{\,i_1-1} \} V \; \ldots\ldots \; V \{ \Sigma_{i_n=0,\infty} R_{i_n}\, y^{\,i_n-1} \}$$

where summation indices are i_0, i_1.....i_n , a total of n+1 indices. This integrand exactly fits our generalized theorem and corollary above, so we may again evaluate the integral "by inspection". The contributing terms all have the same form (n V's and n+1 R's)

$$[\, R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$$

such that the sum of the R indices add up to n ! So we are done with this Kato integral:

$$P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n \; = \; \Sigma_{(n)} \; R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}$$

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

and where the notation $\Sigma_{(n)}$ means "sum over all n+1 indices i_k such that the sum of these indices add up to n".

18. We now turn to the HP integrals. These have an extra factor of z in the integrand, and we would certainly like to turn this into a factor of $(z-E_a^0) = y$ so we have only powers of y to deal with. To this end, let's go back to

$$P = (2\pi i)^{-1} \int_{\Gamma a} dz\, G(z) = \Sigma_{n=0}^{\infty} \lambda^n \, (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n \qquad (8)$$

$$HP = (2\pi i)^{-1} \int_{\Gamma a} dz\, zG(z) = \Sigma_{n=0}^{\infty} \lambda^n \, (2\pi i)^{-1} \int_{\Gamma a} dz\, z\, G_0(VG_0)^n \qquad (9)$$

$$P = \Sigma_{n=0}^{\infty} \lambda^n \, P^{(n)} \qquad P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n$$

$$HP = \Sigma_{n=0}^{\infty} \lambda^n \, (HP)^{(n)} \qquad (HP)^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, z\, G_0(VG_0)^n$$

and let's subtract $E_a^0 P$ from the HP equation (9) to get

$$HP - E_a^0 P = (2\pi i)^{-1} \int_{\Gamma a} dz\, (z- E_a^0) G(z) = \Sigma_{n=0}^{\infty} \lambda^n \, (2\pi i)^{-1} \int_{\Gamma a} dz\, (z- E_a^0)\, G_0(VG_0)^n \qquad (10)$$

$$= \Sigma_{n=0}^{\infty} \lambda^n \, (HP - E_a^0 P)^{(n)}$$

where

$$(HP - E_a^0 P)^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, (z- E_a^0)\, G_0(VG_0)^n = (HP)^{(n)} - E_a^0 P^{(n)}$$

We shall evaluate this last integral using our standard inspection method (modified slightly), and then we can say that

$$(HP)^{(n)} = (HP - E_a^0 P)^{(n)} + E_a^0 P^{(n)}$$

We now evaluate the integral $(2\pi i)^{-1} \int_{\Gamma a} dz\, (z- E_a^0)\, G_0(VG_0)^n$ by inspection as follows. It is exactly the same as our $P^{(n)}$ integral treated above, but there is *one extra factor of y*. Thus, the contributing terms are now those whose y exponents add up to one less than they did before, and that means that the sum of the R_i indices will add up to one less than *they* did before. Before they added up to n, so now they add up to n-1. So here is our conclusion:

$$(HP - E_a^0 P)^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, (z- E_a^0)\, G_0(VG_0)^n = (HP)^{(n)} - E_a^0 P^{(n)}$$

$$= \Sigma_{(n-1)} \, [\, R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$$

$\equiv B^{(n)}$ in Messiah p 717 (71) { we will use this short name later }

using the same Σ notation as above. Therefore, we find that

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

$(HP - E_a^0 P)^{(n)} = \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$

$(HP)^{(n)} = \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] - E_a^0 P^{(n)}$

$= \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}] - E_a^0 \Sigma_{(n)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$

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

In every [..] factor, there are n factors of V, and n+1 factors or R_i .

Let's look at dimensions for a moment. $R_0 = P_0$ is a dimensionless projection operator (as is any projection operator including $Q_0 = 1 - P_0$). The operator $Q_{0a} = Q_0(E_a^0 - H_0)^{-1}Q_0$ has dimensions of 1/energy. Thus, $\dim(R_k) = (\text{energy})^{-k}$.

Each term in the sum for $P^{(n)}$ has dimensions as follows:

$(\text{energy})^{-n} (\text{energy})^{+n} = (\text{energy})^0$

where the second factor comes from the n factors of V, while the first from the R's.

Each term in the sum $(HP - E_a^0 P)^{(n)}$ has these dimensions:

$(\text{energy})^{-(n-1)} (\text{energy})^{+n} = (\text{energy})^1$

as we would expect. Finally, looking at $(HP)^{(n)}$, we see that both terms are $(\text{energy})^1$, again as we would expect.

Compute $P^{(n)}$ for n = 0,1,2,3

19. Remember that n is the number of V factors

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

n=0: R_0

n = 1: $R_1 V R_0 + R_0 V R_1$

n=2: $R_1 V R_1 V R_0 + R_1 V R_0 V R_1 + R_0 V R_1 V R_1$

$+ R_2VR_0VR_0 + R_0VR_2VR_0 + R_0VR_0VR_2$

Since the permutations are pretty obvious, let's start over and just indicate the number of permutations to add to each first term. Remember that n is the number of V's: (see comments below)

n=0: R_0

n=1: R_1VR_0 + 1 perm

n=2: $(R_0VR_1VR_1$ + 2 perms) + $(R_0VR_0VR_2$ + 2 perms)

n=3: $(R_3VR_0VR_0VR_0$ + 3 perms) + $(R_2VR_1VR_0VR_0$ + 11 perms)
+ $(R_1VR_1VR_1VR_0$ + 3 perms)

n=4: $(R_4VR_0VR_0VR_0VR_0$ + 4 perms) + $(R_3VR_1VR_0VR_0VR_0$ + 19 perms)

+ $(R_2VR_2VR_0VR_0VR_0$ + 9 perms) + $(R_2VR_1VR_1VR_0VR_0$ + 29 perms)

+ $(R_1VR_1VR_1VR_1VR_0$ + 4 perms)

There are 19 perms of the second n=4 term as follows: (5,3) = 10 ways to place the three 0's, and for each of these, there are 2 ways to place the 1 and 3. There are 29 permutations of the 4th term as follows: There are (5,2) = 10 ways to place the two 0's, and for each of these ways, there are (3,2) = 3 ways to place the 1's.

Let's now write things out through n=3 in our full notation, where recall

$R_0 \equiv P_0$ and $R_1 = Q_{0a}$ $R_2 = -Q_{0a}^2$ $R_3 = Q_{0a}^3$ etc

Here then are our lowest terms for P (all terms in a permutation group have the same sign)

$P^{(0)} = P_0$

$P^{(1)} = (Q_{0a}V P_0$ + 1 p)

$P^{(2)} = -(Q_{0a}^2VP_0VP_0$ + 2 p) + $(Q_{0a}VQ_{0a}VP_0$ + 2 p)

$P^{(3)} = (Q_{0a}^3VP_0VP_0VP_0$ + 3 p) $-(Q_{0a}^2V\, Q_{0a}VP_0\, VP_0$ + 11 p) + $(Q_{0a}VQ_{0a}VQ_{0a}VP_0$ + 3 p)

Compute $B^{(n)} \equiv (HP - E_a{}^0P)^{(n)}$ and $(HP)^{(n)}$ for n = 0,1,2,3

[It turns out that we don't really need the $(HP)^{(n)}$, just the $B^{(n)}$.]

20. It is easiest to compute the terms for $(HP - E_a^0 P)^{(n)}$ then use $(HP)^{(n)} = (HP - E_a^0 P)^{(n)} + E_a^0 P^{(n)}$, so using the same shorthand notation as above we find: [Note that Messiah on page 717 refers to $(HP - E_a^0 P)^{(n)}$ as simply $B^{(n)}$.

$(HP - E_a^0 P)^{(n)} = \Sigma_{(n-1)} [R_{i_0} V R_{i_1} V \ldots\ldots V R_{i_n}]$ // n = number of V's

n=0: no terms because R_i indices would have to add up to -1

n=1: $R_0 V R_0$

n=2: $(R_1 V R_0 V R_0 +$ 2 perms)

n=3: $(R_2 V R_0 V R_0 V R_0 +$ 3 perms) $+ (R_1 V R_1 V R_0 V R_0 +$ 5 perms)

We can translate this according to our same rule

$R_0 \equiv P_0 \quad R_1 = Q_{0a} \quad R_2 = -Q_{0a}^2 \quad R_3 = Q_{0a}^3$ etc

$(HP - E_a^0 P)^{(0)}$: no terms

$(HP - E_a^0 P)^{(1)}$: $P_0 V P_0$

$(HP - E_a^0 P)^{(2)}$: $(Q_{0a} V P_0 V P_0 +$ 2 perms)

$(HP - E_a^0 P)^{(3)}$: $-(Q_{0a}^2 V P_0 V P_0 V P_0 +$ 3 perms) $+ (Q_{0a} V Q_{0a} V P_0 V P_0 +$5 perms)

So now apply our rule to get the $(HP)^{(n)}$:

$(HP)^{(n)} = (HP - E_a^0 P)^{(n)} + E_a^0 P^{(n)}$

$(HP)^{(0)} = E_a^0 P_0$

$(HP)^{(1)} = P_0 V P_0 + E_a^0 (Q_{0a} V P_0 +$ 1 p)

$(HP)^{(2)} = (Q_{0a} V P_0 V P_0 +$ 2 p) +

$E_a^0 \{ -(Q_{0a}^2 V P_0 V P_0 +$ 2 p) $+ (Q_{0a} V Q_{0a} V P_0 +$ 2 p)$\}$

$(HP)^{(3)} = -(Q_{0a}^2 V P_0 V P_0 V P_0 +$ 3 p) $+ (Q_{0a} V Q_{0a} V P_0 V P_0 +$ 5 p) +

$E_a^0 \{ (Q_{0a}^3 V P_0 V P_0 V P_0 +$ 3 p) $-(Q_{0a}^2 V Q_{0a} V P_0 V P_0 +$ 11 p) $+ (Q_{0a} V Q_{0a} V Q_{0a} V P_0 +$ 3 p) $\}$

Note: In Messiah page 717,

Compute energy corrections for the non-degenerate theory.

21. We begin this section with a few simple mini-theorems:

Theorem 1: $tr(P) = 1 = tr(P_0)$ for the non-degenerate case

Proof: In the simplest basis, P is a diagonal matrix with everything 0 except for a single 1 on the diagonal at the location of the non-degenerate state $|\psi\rangle$ of interest where $H|\psi\rangle = E_a|\psi\rangle$. Thus, sum of diagonal elements = 1. Result is then basis independent since a trace. The exact same proof applies for P_0 using state $|\varphi\rangle$ where $H_0|\varphi\rangle = E_0^a|\varphi\rangle$. Note that $|\psi\rangle \rightarrow |\varphi\rangle$ as $\lambda \rightarrow 0$.

Theorem 2: $HP = E_aP$ for the non-degenerate case

Proof: Apply to state $|\psi\rangle$ and get $H|\psi\rangle = E_a|\psi\rangle$. Apply to all other states and get 0=0. Thus, claim is true as an operator equation.

Theorem 3: $tr(P_0AB) = tr(ABP_0) = tr(BP_0A) = \langle\varphi|AB|\varphi\rangle$ // traces in cyclic order

where $H_0|\varphi\rangle = E_0^a|\varphi\rangle$ and $|\varphi\rangle$ is our non-degenerate state.

Proof: $tr(P_0AB) = tr(BP_0A) = tr(B|\varphi\rangle\langle\varphi|A) = \Sigma_i \langle i| B|\varphi\rangle\langle\varphi|A|i\rangle = \Sigma_i \langle\varphi|A|i\rangle\langle i| B|\varphi\rangle = \langle\varphi| AB |\varphi\rangle$

where we use the fact that $P_0 = |\varphi\rangle\langle\varphi|$ and $1 = \Sigma_i|i\rangle\langle i|$ where all states of H_0 are included in the sum.
[Note that we assume all these states are orthonormal.]

From the first two theorems, we may conclude that

$$tr(HP - E_a^0P) = tr(HP) - tr(E_a^0P) = tr(E_aP) - tr(E_a^0P) = E_a - E_a^0$$

which is the total energy correction due to all powers of λ. Now recall that

$$(HP - E_a^0P) = \Sigma_{n=0}^{\infty} \lambda^n \ (HP - E_a^0P)^{(n)}$$

where

$$(HP - E_a^0P)^{(n)} = \Sigma_{(n-1)} \ [R_{i_0}V R_{i_1}V \ldots\ldots V R_{i_n}] \equiv B^{(n)}$$

Thus we can say

$$E_a - E_a^0 = \Sigma_{n=1}^{\infty} \lambda^n \varepsilon_n = tr(HP - E_a^0P) = tr(\Sigma_{n=0}^{\infty} \lambda^n \ (HP - E_a^0P)^{(n)})$$

$$= \Sigma_{n=0}^{\infty} \lambda^n \ tr(HP - E_a^0P)^{(n)}$$

and thus our n^{th} order energy correction ε_n is simply given by

$$\varepsilon_n = tr[\,(HP - E_a^0 P)^{(n)}\,] = \langle\varphi|\,(HP - E_a^0 P)'^{(n)}\,|\varphi\rangle$$

or shall we say

$$\varepsilon_n = tr[B^{(n)}] = \langle\varphi|B'^{(n)}|\varphi\rangle \qquad // |\varphi\rangle \text{ must be unit normalized}$$

The left equalities follow from the previous equation. The right equalities follows from Theorem 3 where we mean by the notation $B'^{(n)}$ that we have "knocked out" one factor of P_0 in each term in $B^{(n)}$ [which then let's us use Theorem 3] .

For example, we have

$$(HP - E_a^0 P)^{(1)} = B^{(1)} = P_0 V P_0$$

Then to make $B'^{(1)}$, we knock out one of the P_0 factors, so

$$(HP - E_a^0 P)'^{(1)} = B'^{(1)} = V P_0$$

Then we compute:

$$\varepsilon_1 = \langle\varphi|\,B'^{(1)}\,|\varphi\rangle = \langle\varphi|\,V P_0\,|\varphi\rangle = \langle\varphi|V|\varphi\rangle$$

which is a pretty famous result, where we used $P_0|\varphi\rangle = |\varphi\rangle$.

The next case is a little more interesting:

$$(HP - E_a^0 P)^{(2)} = B^{(2)} = (Q_{0a} V P_0 V P_0 + 2 \text{ perms})$$

$$= (Q_{0a} V P_0 V P_0 + P_0 V Q_{0a} V P_0 + P_0 V P_0 V Q_{0a})$$

Then

$$(HP - E_a^0 P)'^{(2)} = B'^{(2)} = (Q_{0a} V P_0 V + P_0 V Q_{0a} V + V P_0 V Q_{0a})$$

where we knocked one P_0 off an end of each term. Then we have

$$\varepsilon_2 = \langle\varphi|\,B'^{(2)}\,|\varphi\rangle = \langle\varphi|\,Q_{0a} V P_0 V + P_0 V Q_{0a} V + V P_0 V Q_{0a}\,|\varphi\rangle$$

$$= \langle\varphi|\,P_0 V Q_{0a} V|\varphi\rangle = \langle\varphi|V Q_{0a} V|\varphi\rangle$$

which is another famous result. Again we used the fact that $P_0|\varphi\rangle = |\varphi\rangle$, and we know that therefore $Q_0|\varphi\rangle = (1\text{-}P_0)\,|\varphi\rangle = 0$ and thus $Q_{0a}|\varphi\rangle = 0$ since $Q_{0a} \equiv Q_0(E_a^0 - H_0)^{-1}Q_0$. So in this situation, any

factor of Q_{0a} which "touches" either $\langle\varphi|$ or $|\varphi\rangle$ kills off that term. So only one of three terms survives.

Just for fun, we can write ε_2 out in more detail to show the meaning of Q_{0a}. In these equations we use $Q_0 = \Sigma_k\ |k\rangle\langle k|$ where this sum is over all states of H_0 except state $|\varphi\rangle$ (sum over the perp space states)

$$\varepsilon_2 = \langle\varphi|VQ_{0a}V|\varphi\rangle = \langle\varphi|V\ Q_0(E_a^0 - H_0)^{-1}Q_0V|\varphi\rangle$$

$$= \langle\varphi|V\ \Sigma_k\ |k\rangle\langle k|(E_a^0 - H_0)^{-1}Q_0V|\varphi\rangle\ = \Sigma_k\langle\varphi|V\ |k\rangle\langle k|(E_a^0 - E_k)^{-1}Q_0V|\varphi\rangle$$

$$= \Sigma_k(E_a^0 - E_k)^{-1}\langle\varphi|V\ |k\rangle\langle k|\ Q_0V|\varphi\rangle\ = \Sigma_k(E_a^0 - E_k)^{-1}\langle\varphi|V\ |k\rangle\langle k|\ V|\varphi\rangle$$

$$= \Sigma_k(E_a^0 - E_k)^{-1}V_{\varphi k}V_{k\varphi}\ = \Sigma_k(E_a^0 - E_k)^{-1}|V_{\varphi k}|^2$$

which is a more traditional form for ε_2. In complicated formulas, we insert this expansion for Q_0 in opportune places within each occurrence of $Q_{0a}{}^k$ and then $(E_a^0 - H_0)^{-k}$ becomes the number $(E_a^0 - E_k)^{-k}$ and we end up with a formula with one perp space sum for each isolated $Q_{0a}{}^k$ factor.

Before trying the ε_3 term, let's look once more at this knock-out business. A "term" always begins and ends with a P_0 or with a Q_{0a}. So there are *four types of terms*:

$P_0V....VP_0$ $\quad$ $Q_{0a}\ V....VP_0$ $\quad$ $P_0V....V\ Q_{0a}$ $\quad$ $Q_{0a}\ V....V\ Q_{0a}$

We know, by the way, that terms of the last type will have a P_0 internal somewhere, because that is the nature of the terms in $B^{(n)}$. For the moment, let's ignore the fourth term type and look at the first three. In all three cases, we see the P_0 we are going to knock out on one end or the other. In terms of the matrix element $\langle\varphi|\ B'^{(n)}|\varphi\rangle$ [where prime means we have done the knock out] , knocking out an *ending* P_0 has no effect on the matrix element, since $P_0|\varphi\rangle\ = |\varphi\rangle$ anyway. So for the first three term types, when we take the knocked-out matrix element, it is the same as the non-knocked-out matrix element, and thus we see at once that only the first of the three term types can survive because of the ending Q_{0a} factors.

So let's start over and dismiss the two central types of terms shown above, so we only need to worry about these two types of terms:

$P_0V....VP_0$ $\quad$ $Q_{0a}\ V....V\ Q_{0a}$

For the first term type we will say this

$$tr(P_0V....VP_0) = \langle\varphi|\ V....VP_0|\varphi\rangle \qquad \text{// knocking out the left } P_0$$

$$= \langle\varphi|\ V....V|\varphi\rangle$$

What happens with the other term type? Imagine it has this form

$$Q_{0a}\ VAP_0BV\ Q_{0a}$$

where we know that somewhere inside is at least one factor of P_0 and we have here exposed one such factor. For this term we would have

$$\mathrm{tr}(Q_{0a}VAP_0BVQ_{0a}) = \langle\varphi|\ (BVQ_{0a})(Q_{0a}VA)|\varphi\rangle \qquad \text{since} \qquad \mathrm{tr}(bP_0a) = \langle\varphi|ab|\varphi\rangle$$

where the key fact here is that we have to reverse order of b and a when P_0 appears out in the middle somewhere. Thus, we find that

$$\mathrm{tr}(Q_{0a}VAP_0BVQ_{0a}) = \langle\varphi|\ BVQ_{0a}^2VA|\varphi\rangle$$

This term will be non-zero if the leftmost end of B and the rightmost end of A is a P_0! Notice that it would have been a mistake to take the initial term type Q_{0a} V....V Q_{0a} and throw it out before doing the knockout, based on the fact that each end has a Q_{0a}.

Now let's apply this logic to our n=3 terms:

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

Let's abbreviate $Q_{0a} = 1$ and $P_0 = 0$ and write out these terms symbolically as

$$B^{(3)} = -(1^2000 + 01^200 + 001^20 + 0001^2) + (1100 + 1010 + 1001 + 0110 + 0101 + 0011)$$

We now throw out all terms which have a 1 *just one* of the two ends

$$B^{(3)} \approx -(01^200 + 001^20) + (1001 + 0110)$$

$$= -(P_0VQ_{0a}^2VP_0V + P_0VP_0VQ_{0a}^2V) + (P_0VQ_{0a}VQ_{0a}VP_0) + (Q_{0a}VP_0V\ P_0VQ_{0a})$$

Ignoring the last term which is of class 4, the other terms yield

$$\mathrm{tr}(\text{first terms}) = \langle\varphi| -(P_0VQ_{0a}^2VP_0V + P_0VP_0VQ_{0a}^2V) + (P_0VQ_{0a}VQ_{0a}VP_0)|\varphi\rangle$$

$$= \langle\varphi| - VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V + VQ_{0a}VQ_{0a}V|\varphi\rangle$$

For the last term 1001, we select one of the internal P_0 to knock out, and we get

$$\mathrm{tr}(Q_{0a}VP_0V\ P_0VQ_{0a}) = \langle\varphi|\ VP_0VQ_{0a}Q_{0a}V\ |\varphi\rangle = \langle\varphi|\ VP_0VQ_{0a}^2V\ |\varphi\rangle$$

Thus our total result from all four terms is this

$$= \langle\varphi| - VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V + VQ_{0a}VQ_{0a}V + VP_0VQ_{0a}^2V\ |\varphi\rangle$$

and we see that two terms cancel, giving us this final result

$$tr(B'^{(3)}) = \langle\varphi| - VQ_{0a}^2VP_0V + VQ_{0a}VQ_{0a}V |\varphi\rangle$$

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

and this (finally!) agrees with Messiah page 717 (74).

We have dutifully followed the prescription of "knocking out" one end factor of P_0. In retrospect, this only makes a difference with terms of the fourth type considered above.

The conclusion here is that the Kato expansion method allows for a systematic evaluation of the energy correction of a degenerate state to arbitrary order. Based on our previous paragraph, the operative formula is this:

$$\varepsilon_n = tr[\, B^{(n)}\,] = \langle\varphi|B'^{(n)}|\varphi\rangle \quad \text{where} \quad B^{(n)} = \Sigma_{(n-1)}\ [\, R_{i_0}V\, R_{i_1}V \,.....\, V\, R_{i_n}]$$

and where the prime means we have knocked out a P_0 in each subterm of $B^{(n)}$.

It is a completely mechanical process to do the combinatorics to compute $B^{(n)}$, we then throw out non-contributing terms, and get our result as a sum of terms of the form $\langle\varphi|$ ....$|\varphi\rangle$ wherein we shall find exactly n factors of V (corresponding to λ^n) , and n-1 factors of either Q_{0a} or P_0 , where these will only occupy interior positions shielded from the bra and ket by V operators. Any interior P_0 gets replaced by $|\varphi\rangle\langle\varphi|$, and for calculation any interior Q_{0a} gets replaced by itself times the perp space sum $Q_0 = \Sigma_k$ $|k\rangle\langle k|$ which then allows evaluation of each term as one or more sums over k. There is no need to compute the state corrections in this method, as there is in the traditional iterative method which is presented earlier in Messiah's Chapter 16.

The main power of the Kato method, however, comes in solving the degenerate problem! This method is reviewed in detail in our Round Two Resolvent notes, but here we give a summary.

The Degenerate Case with Kato

In the case that E_a^0 is a degenerate eigenvalue of H_0 things are more complicated. We end up with a sequence of "generalized" eigenvalue equations as we go to each higher order in λ. To all orders, the eigenvalue equation is this:

$$H_a\ |\mathcal{E}_a^0\alpha\rangle = E_\alpha\, K_a\ |\mathcal{E}_a^0\alpha\rangle$$

where H_a and K_a are defined as

$$H_a \equiv P_0HPP_0 \qquad K_a \equiv P_0PP_0$$

where we see the presence of our HP and P operators, for which we now have λ expansions due to all our work done above. For example, we have

$$P = \Sigma_{n=0}^{\infty}\, \lambda^n\ P^{(n)} \qquad P^{(n)} \equiv (2\pi i)^{-1} \int_{\Gamma a} dz\, G_0(VG_0)^n$$

$$HP = \Sigma_{n=0}^{\infty} \lambda^n \ (HP)^{(n)} \qquad\qquad (HP)^{(n)} \equiv \ (2\pi i)^{-1} \int_{\Gamma a} dz \ z \ G_0(VG_0)^n$$

and we computed the integrals above to be

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

$$(HP - E_a^0 P)^{(n)} = \Sigma_{(n-1)} \ [R_{i_0} V R_{i_1} V \ ..... \ V R_{i_n}]$$

$$(HP)^{(n)} \ = (HP - E_a^0 P)^{(n)} \ + E_a^0 \ P^{(n)}$$

Thus we can write

$$H_a \equiv P_0 H P P_0 = \Sigma_{n=0}^{\infty} \lambda^n \ P_0 \ (HP)^{(n)} P_0$$

$$K_a \equiv P_0 P P_0 = \Sigma_{n=0}^{\infty} \lambda^n \ P_0 \ P^{(n)} P_0$$

$$E_\alpha = E_a^0 + \Sigma_{n=1}^{\infty} \lambda^n \varepsilon_n$$

According to my Pause for Comments in the Round Two resolvent doc, you have to think of the above equation in the sense of "through some order", not "in" a particular order.

Here is possible way to do things:

$$H_a \equiv P_0 H P P_0 \qquad K_a \equiv P_0 P P_0$$

$$L_a \equiv P_0 (HP - E_a^0 P) P_0 \ = \ P_0 B P_0 \qquad\qquad B = (HP - E_a^0 P)$$

$$H_a \ = L_a + E_a^0 \ P_0 P P_0 \ = L_a + E_a^0 \ K_a$$

Our EV equation then becomes

$$H_a \ |\mathcal{E}_a^0 \alpha\rangle = E_\alpha \ K_a \ |\mathcal{E}_a^0 \alpha\rangle \ = (L_a + E_a^0 \ K_a) \ |\mathcal{E}_a^0 \alpha\rangle$$

or

$$L_a |\mathcal{E}_a^0 \alpha\rangle = (E_\alpha - E_a^0) \ K_a \ |\mathcal{E}_a^0 \alpha\rangle$$

Now maybe here are better names for our operators

$K_a = P' = P_0 P P_0$ // P sandwiched by P_0's

$L_a = B' = P_0 B P_0$ // B sandwiched by P_0's

Then our EV equation becomes

$$B'|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\, P'\, |\mathcal{E}_a^0\alpha\rangle$$

Now let's look at this thing through various orders. But first, let's collect our data right here:

$$P^{(0)} = P_0$$
$$P^{(1)} = (Q_{0a} V P_0 + 1\ p)$$
$$P^{(2)} = -(Q_{0a}^2 V P_0 V P_0 + 2\ p) + (Q_{0a} V Q_{0a} V P_0 + 2\ p)$$
$$P^{(3)} = (Q_{0a}^3 V P_0 V P_0 V P_0 + 3\ p) - (Q_{0a}^2 V\, Q_{0a} V P_0\, V P_0 + 11\ p) + (Q_{0a} V Q_{0a} V Q_{0a} V P_0 + 3\ p)$$

$B^{(0)}$: 0
$B^{(1)}$: $P_0 V P_0$
$B^{(2)}$: $(Q_{0a} V P_0 V P_0 + 2 \text{ perms})$
$B^{(3)}$: $-(Q_{0a}^2 V P_0 V P_0 V P_0 + 3 \text{ perms}) + (Q_{0a} V Q_{0a} V\, P_0 V P_0 + 2 \text{ perms})$

We can do some precomputation here with our usual rules for throwing things out:

$$P'^{(0)} = P_0$$
$$P'^{(1)} = 0$$
$$P'^{(2)} = -(P_0 V\, Q_{0a}^2 V P_0)$$
$$P'^{(3)} = (P_0 V Q_{0a}^3 V P_0 V P_0 + P_0 V P_0 V Q_{0a}^3 V P_0) - (P_0 V Q_{0a}^2 V\, Q_{0a} V\, P_0 + P_0 V Q_{0a} V\, Q_{0a}^2 V\, P_0)$$

In the above, we deleted all terms with a Q_0 on either end. Similarly we get

$B'^{(0)}$: 0
$B'^{(1)}$: $P_0 V P_0$
$B'^{(2)}$: $(P_0 V Q_{0a} V P_0)$
$B'^{(3)}$: $-(P_0 V Q_{0a}^2 V P_0 V P_0 + P_0 V P_0 V Q_{0a}^2 V P_0) + (P_0 V Q_{0a} V Q_{0a} V\, P_0)$

Then we can just write :

$$P' = P_0 - \lambda^2 (P_0 V\, Q_{0a}^2 V P_0) + \lambda^3 \{ (P_0 V Q_{0a}^3 V P_0 V P_0 + P_0 V P_0 V Q_{0a}^3 V P_0) - (P_0 V Q_{0a}^2 V\, Q_{0a} V\, P_0 + P_0 V Q_{0a} V\, Q_{0a}^2 V\, P_0)\}$$

$$B' = \lambda\, P_0 V P_0 + \lambda^2 P_0 V Q_{0a} V P_0 + \lambda^3 \{ -(P_0 V Q_{0a}^2 V P_0 V P_0 + P_0 V P_0 V Q_{0a}^2 V P_0) + (P_0 V Q_{0a} V Q_{0a} V\, P_0) \}$$

$$B'|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\, P'\, |\mathcal{E}_a^0\alpha\rangle$$

The Level 1 Problem.

I will here install B' through order λ^1 on the LHS. Since $(E_\alpha - E_a^0)$ is itself order λ, I will only install P' through order λ^0. Thus:

$$B'|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\, P'\, |\mathcal{E}_a^0\alpha\rangle$$

$\lambda\, P_0 V P_0' |\mathcal{E}_a^0 \alpha\rangle = (E_\alpha - E_a^0)\, P_0\, |\mathcal{E}_a^0 \alpha\rangle$

Identify the energy difference with $\lambda\varepsilon_1$ and do the usual so this becomes

$$V|\mathcal{E}_a^0 \alpha\rangle = \varepsilon_1 |\mathcal{E}_a^0 \alpha\rangle$$

which is the traditional result.

The Level 2 Problem.

I will here install B' through order λ^2 on the LHS. Since $(E_\alpha - E_a^0)$ is itself order λ, I will only install P' through order λ^1. Thus:

$B'|\mathcal{E}_a^0 \alpha\rangle = (E_\alpha - E_a^0)\, P'\, |\mathcal{E}_a^0 \alpha\rangle$

$\{ \lambda P_0 V P_0 + \lambda^2 P_0 V Q_{0a} V P_0 \} |\mathcal{E}_a^0 \alpha\rangle = (E_\alpha - E_a^0) \{ P_0 \} |\mathcal{E}_a^0 \alpha\rangle$

$\{ \lambda V + \lambda^2 V Q_{0a} V \} |\mathcal{E}_a^0 \alpha\rangle = (E_\alpha - E_a^0) |\mathcal{E}_a^0 \alpha\rangle$

$\{ \lambda V + \lambda^2 V Q_{0a} V \} |\mathcal{E}_a^0 \alpha\rangle = (\lambda\varepsilon_1 + \lambda^2\varepsilon_2 + \lambda^3\varepsilon_3 + ...) |\mathcal{E}_a^0 \alpha\rangle$

This is the equation we would solve to find exact eigenvalues $(E_\alpha - E_a^0)$ as f(λ), which we could Taylor expand f(λ) as shown. We would also find the exact eigenkets $|\mathcal{E}_a^0 \alpha\rangle$ for the above problem. Now suppose we try to write the above single equation as two equations by "matching powers of λ". I think the right thing to say is this:

$\lambda V |\mathcal{E}_a^0 \alpha\rangle = \lambda\varepsilon_1 |\mathcal{E}_a^0 \alpha\rangle$ + order(λ^2) and higher

$\lambda^2 V Q_{0a} V |\mathcal{E}_a^0 \alpha\rangle = \lambda^2\varepsilon_2 |\mathcal{E}_a^0 \alpha\rangle$ + order(λ^3) and higher

So neither of these equations is an exact EV equation. Only the full equation written above is the real EV equation. BUT, our second equation here is an *approximate* EV equation if we throw out order λ^3 and above. Similarly, the first equation is an approximate EV equation of we through out order λ^2 and above. These two approximate EV equations of course have different solutions $|\mathcal{E}_a^0 \alpha\rangle$! If we are interested in computing the eigenenergies only, we can deal with these approximate equations, but if we want to know that true states $|\mathcal{E}_a^0 \alpha\rangle$, we have to do the full equation, which with λ = 1 we write as

$$\{ V + V Q_{0a} V \} |\mathcal{E}_a^0 \alpha\rangle = \Delta E_\alpha |\mathcal{E}_a^0 \alpha\rangle \qquad \Delta E_\alpha = (E_\alpha - E_a^0)$$

I would call this a well-defined eigenvalue problem that one would actually solve for eigenvalues and eigenkets. In particular:

$$\det(V + V Q_{0a} V - \Delta E_\alpha 1) = 0$$

gives the eigenenergies. It is not clear to me how the eigenvalues so obtained would compare to the sum of the eigenvalues of the two approximate EV equations shown above. Would we find that

$$\Delta E_\alpha \approx \lambda\varepsilon_1 + \lambda^2\varepsilon_2 \quad ?$$

Another view of the Level 2 problem. Suppose we solve the Level 1 problem $V|\mathcal{E}_a^0\alpha\rangle = \varepsilon_1|\mathcal{E}_a^0\alpha\rangle$, and suppose we find that all N eigenvalues are the same, so that we still have N degenerate kets. This would be the case for example if V were a multiple of the identity matrix. In this case, *any* set of kets $|\mathcal{E}_a^0\alpha\rangle$ in the space $\mathcal{E}_a^0$ would be eigenkets of V. And in this radical case, $VQ_{0a}V = k\,Q_{0a}$ and this would vanish against $|\mathcal{E}_a^0\alpha\rangle$ and then our whole pyramid collapses into nothing.

Now suppose instead we solve the Level 1 problem and find that at least one subset of the kets are still degenerate, so we still have some M degenerate kets (perhaps several sets, but focus on one set). Of course M < N now. How would this situation affect our Level 2 problem as stated above?

$$\{ V + VQ_{0a}V\}\,|\mathcal{E}_a^0\alpha\rangle = \Delta E_\alpha\,|\mathcal{E}_a^0\alpha\rangle \qquad \Delta E_\alpha = (E_\alpha - E_a^0)$$

If we now restrict $|\mathcal{E}_a^0\alpha\rangle$ to this M dimensional subspace, I think we can say that

$$V|\mathcal{E}_a^0\alpha\rangle = \varepsilon_1|\mathcal{E}_a^0\alpha\rangle \qquad \text{and in fact} \qquad V = \varepsilon_1 \text{ as an operator on this subspace}$$

Then our full Level 2 problem says:

$$\{ \varepsilon_1 + VQ_{0a}V\}\,|\mathcal{E}_a^0\alpha\rangle = \Delta E_\alpha\,|\mathcal{E}_a^0\alpha\rangle$$

$$(VQ_{0a}V)\,|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0 - \varepsilon_1)\,|\mathcal{E}_a^0\alpha\rangle = K_i\,|\mathcal{E}_a^0\alpha\rangle \qquad \text{// See Messiah p 700 (39)}$$

This is now an exact MxM eigenvalue problem which we could then solve for M eigenvalues K_i. In the last equation above, ε_1 is the common eigenvalue of all M states in the Level 1 problem, it is a single well-defined real number. Our secular equation is then

$$\det[VQ_{0a}V - (E_\alpha - E_a^0 - \varepsilon_1)\,1] = 0$$

which gives us a polynomial of degree M in the quantity $(E_\alpha - E_a^0 - \varepsilon_1)$.

We might then find that even after Level 2, we still have a degenerate subspace of some dimension J < M < N. Then I think we would look at the Level 3 problem. See below.

The Level 3 Problem.

I will here install B' through order λ^3 on the LHS. Since $(E_\alpha - E_a^0)$ is itself order λ, I will only install P' through order λ^2. Thus:

$$P' = P_0 - \lambda^2 (P_0 V\, Q_{0a}^2 V P_0)$$

$$B' = \lambda P_0 V P_0 + \lambda^2 P_0 V Q_{0a} V P_0 + \lambda^3 \{ -(P_0 V Q_{0a}^2 V P_0 V P_0 + P_0 V P_0 V Q_{0a}^2 V P_0) + (P_0 V Q_{0a} V Q_{0a} V P_0) \}$$

$$B'|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0) P' |\mathcal{E}_a^0\alpha\rangle$$

Let's pre-remove the P_0 on each end of everything

$$P' = 1 - \lambda^2 (V Q_{0a}^2 V)$$

$$B' = \lambda V + \lambda^2 V Q_{0a} V + \lambda^3 \{ -(V Q_{0a}^2 V P_0 V + V P_0 V Q_{0a}^2 V) + (V Q_{0a} V Q_{0a} V) \}$$

And next, set $\lambda = 1$ and do out the signs: (but remember each V is order λ)

$$P' = 1 - V Q_{0a}^2 V$$

$$B' = V + V Q_{0a} V - V Q_{0a}^2 V P_0 V - V P_0 V Q_{0a}^2 V + V Q_{0a} V Q_{0a} V \}$$

$$B'|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0) P' |\mathcal{E}_a^0\alpha\rangle$$

$$\{ V + V Q_{0a} V - V Q_{0a}^2 V P_0 V - V P_0 V Q_{0a}^2 V + V Q_{0a} V Q_{0a} V \} |\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\{ 1 - V Q_{0a}^2 V\} |\mathcal{E}_a^0\alpha\rangle$$

Now this equation maintains the "generalized eigenvalue problem form", unlike our Level 1 problem. I don't know how to solve this, or whether $\{ 1 - V Q_{0a}^2 V\}$ has an inverse (probably not). But in principle this kind of problem can be solved and we would end up with eigenvalues for $(E_\alpha - E_a^0)$ and eigenkets of the form $|\mathcal{E}_a^0\alpha\rangle$. Imagine the λ's still in place. We then have an equation of this form:

$$\{ A\lambda + B\lambda^2 + C\lambda^3 + ...\} |\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\{ 1 + \lambda^2 D .....\} |\mathcal{E}_a^0\alpha\rangle$$

Since $(E_\alpha - E_a^0) \sim \lambda$, we see that "the next terms" on each side would be order λ^4. Suppose we expanded the eigenvalue in a power series in the usual way, so then we have

$$\{ A\lambda + B\lambda^2 + C\lambda^3 + ...\} |\mathcal{E}_a^0\alpha\rangle = [\lambda\varepsilon_1 + \lambda^2\varepsilon_2 + \lambda^3\varepsilon_3 + ...] \{ 1 + \lambda^2 D .....\} |\mathcal{E}_a^0\alpha\rangle$$

Notice that the term $\lambda^3\varepsilon_3 \{ 1\} |\mathcal{E}_a^0\alpha\rangle$ makes an order λ^3 contribution on the RHS, so it's presence is felt through this order. So I think I want to claim that if you could solve this equation, you would have a good estimate for the energy correction through λ^3 order. It is not totally obvious how you make this claim.

Now let's try our little test question again. Suppose we have a subspace of dimension $J < M < N$ which is still degenerate after our level 2 processing. Then in the subspace of the J's, we have

$$\{ V + V Q_{0a} V\} |\mathcal{E}_a^0\alpha\rangle = \Delta E_{\alpha,2} |\mathcal{E}_a^0\alpha\rangle$$

where $\Delta E_{\alpha,2}$ is the same number for all J eigenvectors in this space. Thus, if we restrict to the J space, we should be able to replace $V + VQ_{0a}V$ with the number $\Delta E_{\alpha,2}$ that we found by solving the level 2 problem. This is a unique number for this subspace. Then our Level 3 equation becomes:

$$\{ V + VQ_{0a}V \ -VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V \ + VQ_{0a}VQ_{0a}V \}|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\{ 1- VQ_{0a}^2V\}|\mathcal{E}_a^0\alpha\rangle$$

$$\{ \Delta E_{\alpha,2} \ -VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V \ + VQ_{0a}VQ_{0a}V \}|\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\{ 1- VQ_{0a}^2V\}|\mathcal{E}_a^0\alpha\rangle$$

Perhaps this makes the equation slightly simpler. Could also write as

$$\Delta E_{\alpha,2}|\mathcal{E}_a^0\alpha\rangle + V\{ -Q_{0a}^2VP_0 - P_0VQ_{0a}^2 \ + Q_{0a}VQ_{0a}\}V \ |\mathcal{E}_a^0\alpha\rangle = (E_\alpha - E_a^0)\{ 1- VQ_{0a}^2V\}|\mathcal{E}_a^0\alpha\rangle$$

I guess I really need to look at Kato someday to see how this is handled. Even without solving it, we could at least find $(E_\alpha - E_a^0)$ through third order using our secular equation:

$$\det [\Delta E_{\alpha,2} \ -VQ_{0a}^2VP_0V - VP_0VQ_{0a}^2V \ + VQ_{0a}VQ_{0a}V - \ (E_\alpha - E_a^0)\{ 1- VQ_{0a}^2V\} \ ] = 0$$

This would still be a polynomial of degree J in the quantity $(E_\alpha - E_a^0)$.

In theory, we can write out our EV to any order we want and try to solve it. We can always write the secular equation in any order, although the number of terms is going to increase fast.

Kato has at least given us a framework in which we can attempt to solve nasty degeneracy problems, and in theory we could do it through perhaps 4th or 5th order without breaking the bank.