HIGHER-ORDER SPECTRAL PERTURBATION

by a new determinantal method

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September 2000

Introduction. Recently I had occasion to describe[1] a method for computing the energy spectrum

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots \tag{1}$$

of a perturbed quantum system

$$\mathsf{H} = \mathsf{H}^0 + \lambda \mathsf{V}$$

which—in sharp contrast to the familiar Rayleigh-Schrödinger method—proceeds entirely without reference to the perturbed eigenvectors

$$|n) = |n^0) + \lambda|n^1) + \lambda^2|n^2) + \cdots$$

The method was used to reproduce the standard formulæ

$$E_n^1 = (n^0|\mathsf{V}|n^0) \quad : \text{ abbreviated } \quad V_{nn} \tag{2.1}$$

$$E_n^2 = -\sum_{m\neq n} \frac{(n^0|\mathsf{V}|m^0)(m^0|\mathsf{V}|n^0)}{E_m^0 - E_n^0} \quad : \text{ abbreviated } \quad -\sum_{i\neq n}\frac{V_{ni}V_{in}}{D_{in}} \tag{2.2}$$

and to produce (at (A23.3)) a formula

$$E_n^3 = \sum_{i,j\neq n} \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}} - E_n^1 \cdot \sum_{i\neq n} \frac{V_{ni}V_{in}}{D_{in}^2} \tag{2.3}$$

which I had been unable to discover in the literature, but which Oz Bonfim has today informed me is posed as Problem 2 on page 136 of the 3rd edition of Landau & Lifshitz' *Quantum Mechanics* (it is absent from my 2nd edition). Oz's research has stimulated an interest in E_n^4, and it is at his request that I return to this subject.

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[1] "Perturbed spectra without pain," (April 2000). I refer in these pages to that essay as Part A.

In the unperturbed eigenbasis the matrix

$$\mathbb{H}^0 \equiv \|(m^0|\mathsf{H}^0|n^0)\| \quad \text{is diagonal}$$

and its diagonal elements E_n^0 are presumed to be known. Also assumed in each instance to be known are the matrix elements of

$$\mathbb{V} \equiv \|(m^0|\mathsf{H}^0|n^0)\| \equiv \|V_{mn}\|$$

Initially we assume the unperturbed spectrum $\{E_n^0\}$ to be non-degenerate, but the method will ultimately permit that assumption to be relaxed. We take as our assignment the development (1) of the roots of the equation

$$\det\big\{\mathbb{H}^0 + \lambda\mathbb{V} - E\,\mathbb{I}\,\big\} = 0 \tag{3}$$

which in Part A I contrive to accomplish in a way which makes sense even when the matrices are ∞-dimensional, and the characteristic polynomial a "polynomial of ∞ order."

Pattern of the argument, stripped of distracting details. Write

$$\det\big\{\mathbb{H}^0 + \lambda\mathbb{V} - E\,\mathbb{I}\big\} = \det\big\{\mathbb{H}^0 - E\,\mathbb{I}\big\}\cdot\det\big\{\mathbb{I} + \lambda\mathbb{M}\big\} \tag{4}$$

$$\mathbb{M} \equiv (\mathbb{H}^0 - E\,\mathbb{I})^{-1}\,\mathbb{V}$$

$$\det\big\{\mathbb{H}^0 - E\,\mathbb{I}\big\} = \prod_i (E_i^0 - E)$$

and observe that the first factor, regarded as a function of E, has zeros at precisely the (unperturbed spectral) points were the second factor becomes singular; evidently some delicate cancellations must come into play if the product is to vanish at *perturbed* spectral points.

Formal expansion of[2]

$$P(E) \equiv \prod_i (E_i^0 - \underset{\substack{\uparrow \\ E\,=\,E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots}}{E})$$

is straightforward in principle, but leads to an instance of the "partition problem"—therefore to a superabundance of terms even in low order; one obtains a result of the form

$$\begin{aligned} P(E) &= P(E^0) + \lambda P(E^0, E^1) + \lambda^2 P(E^0, E^1, E^2) + \cdots \\ &\equiv P_0 + \lambda P_1 + \lambda^2 P_2 + \cdots \end{aligned} \tag{5}$$

[2] It will be my practice to omit the subscript $_n$ from (1) in generic situations.

Expansion of $\det\{\mathbb{I}+\lambda\mathbb{M}\}$ is accomplished by appeal to an identity as pretty as it is little known (and which makes formal sense even in the infinite dimensional case):

$$\det\{\mathbb{I}+\lambda\mathbb{M}\} = 1+\lambda T_1 + \tfrac{1}{2!}\lambda^2\begin{vmatrix} T_1 & T_2\\ 1 & T_1\end{vmatrix} + \tfrac{1}{3!}\lambda^3\begin{vmatrix} T_1 & T_2 & T_3\\ 1 & T_1 & T_2\\ 0 & 2 & T_1\end{vmatrix} + \tfrac{1}{4!}\lambda^4\begin{vmatrix} T_1 & T_2 & T_3 & T_4\\ 1 & T_1 & T_2 & T_3\\ 0 & 2 & T_1 & T_2\\ 0 & 0 & 3 & T_1\end{vmatrix}+\cdots \tag{6.1}$$

$$\equiv \Delta_0 + \lambda\Delta_1 + \tfrac{1}{2!}\lambda^2\Delta_2 + \tfrac{1}{3!}\lambda^3\Delta_3 + \tfrac{1}{4!}\lambda^4\Delta_4+\cdots \tag{6.2}$$

where direct evaluation of the determinants (or appeal to a recursion relation that need not concern us) gives

$$\left.\begin{aligned}
\Delta_0 &= 1\\
\Delta_1 &= T_1\\
\Delta_2 &= T_1^2 - T_2\\
\Delta_3 &= T_1^3 - 3T_1T_2 + 2T_3\\
\Delta_4 &= T_1^4 - 6T_1^2T_2 + 8T_1T_3 + 3T_2^2 - 6T_4\\
\Delta_5 &= T_1^5 - 10T_1^3T_2 + 20T_1^2T_3 + 15T_1(T_2^2-4T_4) - 20T_2T_3 + 24T_5\\
&\ \ \vdots
\end{aligned}\right\} \tag{7}$$

with $T_p \equiv \operatorname{tr}\mathbb{M}^p$.

We confront now the awkward fact that

$$\mathbb{M} = \left\|\frac{V_{ij}}{E_i - E}\right\| \quad \text{acquires } \lambda\text{-dependence from } E \tag{8}$$

So each T_p also does, and so finally does each Δ_k. Suppose we *were* in possession of the trace expansions

$$T_p = T_{p0} + \lambda T_{p1} + \lambda^2 T_{p2} + \cdots \tag{9}$$

Insertion of those into (7), and of the results into (6.2), yields a series of the form

$$\det\{\mathbb{I}+\lambda\mathbb{M}\} = 1 + \lambda Q_1 + \lambda^2 Q_2 + \cdots \tag{10}$$

where, according to *Mathematica*,

$$Q_1 = T_{10} \tag{11.1}$$

$$Q_2 = \tfrac{1}{2}\big[T_{10}^2 - T_{20} + 2T_{11}\big] \tag{11.2}$$

$$Q_3 = \tfrac{1}{6}\big[T_{10}^3 + 6T_{12} + T_{10}(6T_{11} - 3T_{20}) - 3T_{21} + 2T_{30}\big] \tag{11.3}$$

$$\begin{aligned} Q_4 = \tfrac{1}{24}\big[&T_{10}^4 + 12T_{11}^2 + 24T_{13} + 6T_{10}^2(2T_{11} - T_{20}) - 12T_{11}T_{20} \\ &+ 3T_{20}^2 - 12T_{22} + 4T_{10}(6T_{12} - 3T_{21} + 2T_{30}) + 8T_{31} - 6T_{40}\big] \end{aligned} \tag{11.4}$$

$$\begin{aligned} Q_5 = \tfrac{1}{120}\big[&T_{10}^5 + 10T_{10}^3(2T_{11} - T_{20}) + 10T_{10}^2(6T_{12} - 3T_{21} + 2T_{30}) \\ &+ 5T_{10}(12T_{11}^2 + 24T_{13} - 12T_{11}T_{20} + 3T_{20}^2 - 12T_{22} + 8T_{31} - 12T_{40}) \\ &+ 120T_{14} - 60T_{12}T_{20} + 30T_{20}T_{21} - 60T_{23} - 20T_{20}T_{30} \\ &+ 20T_{11}(6T_{12} - 3T_{21} + 2T_{30}) + 40T_{32} - 30T_{41} + 24T_{50}\big] \end{aligned} \tag{11.5}$$

$$\vdots$$

Multiplication of (5) into (10) gives

$$\begin{aligned} \det\big\{\mathbb{H}^0 + \lambda\mathbb{V} - E\,\mathbb{I}\big\} = P_0 &+ \lambda\ \big(P_1 + P_0Q_1\big) \\ &+ \lambda^2\big(P_2 + P_1Q_1 + P_0Q_2\big) \\ &+ \lambda^3\big(P_3 + P_2Q_1 + P_1Q_2 + P_0Q_3\big) \\ &+ \lambda^4\big(P_4 + P_3Q_1 + P_2Q_2 + P_1Q_3 + P_0Q_4\big) \\ &+ \lambda^5\big(P_5 + P_4Q_1 + P_3Q_2 + P_2Q_3 + P_1Q_4 + P_0Q_5\big) \end{aligned}$$

and to achieve (3) we must have

$$P_0 = 0 \tag{12.0}$$

$$P_1 + P_0Q_1 = 0 \tag{12.1}$$

$$P_2 + P_1Q_1 + P_0Q_2 = 0 \tag{12.2}$$

$$P_3 + P_2Q_1 + P_1Q_2 + P_0Q_3 = 0 \tag{12.3}$$

$$P_4 + P_3Q_1 + P_2Q_2 + P_1Q_3 + P_0Q_4 = 0 \tag{12.4}$$

$$P_5 + P_4Q_1 + P_3Q_2 + P_2Q_3 + P_1Q_4 + P_0Q_5 = 0 \tag{12.5}$$

$$\vdots$$

The left side of (12.0) presents only E^0 as an argument, and forces us to set

$$E^0 = \text{one of the unperturbed eigenvalues, call it } E_n^0 \tag{13}$$

The left side of (12.1) presents E^0, E^1: solve for E^1 (i.e., for E_n^1).
The left side of (12.1) presents E^0, E^1, E^2: solve for E^2 (i.e., for E_n^2).

So it goes if E_n^0 is non-degenerate. As it turns out, the adjustments required in the contrary case are made obvious by the detailed design of equations (12).

Construction of the P-coefficients. The objects of present interest arose at (5), where we had

$$\prod_i (E_i^0 - E^0 - \lambda E^1 - \lambda^2 E^2 - \cdots) \equiv P_0 + \lambda P_1 + \lambda^2 P_2 + \cdots$$

Evidently

$$P_0 = \prod_i (E_i^0 - E^0) \ : \ \text{also called } \Pi_0 \tag{14.0}$$

$$P_1 = -E^1\Pi_1 \tag{14.1}$$

$$P_2 = -E^2\Pi_1 + E^1E^1\Pi_2 \tag{14.2}$$

$$P_3 = -E^3\Pi_1 + \mathbf{2}E^2E^1\Pi_2 - E^1E^1E^1\Pi_3 \tag{14.3}$$

$$P_4 = -E^4\Pi_1 + (\mathbf{2}E^3E^1 + E^2E^2)\Pi_2 - \mathbf{3}E^2E^1E^1\Pi_3 + E^1E^1E^1E^1\Pi_4 \tag{14.4}$$

$$\begin{aligned} P_5 = -E^5\Pi_1 &+ (\mathbf{2}E^4E^1 + \mathbf{2}E^3E^2)\Pi_2 - (\mathbf{3}E^3E^1E^1 + \mathbf{3}E^2E^2E^1)\Pi_3 \\ &+ \mathbf{4}E^2E^1E^1E^1\Pi_4 - E^1E^1E^1E^1E^1\Pi_5 \end{aligned} \tag{14.5}$$

$$P_6 = \text{etc.}$$

where

$$\begin{aligned} \Pi_1(E^0) &\equiv \text{sum over all ways of striking one factor from } P_0 \\ \Pi_2(E^0) &\equiv \text{sum over all distinct ways of striking two factors from } P_0 \\ \Pi_3(E^0) &\equiv \text{sum over all distinct ways of striking three factors from } P_0 \\ &\ \vdots \end{aligned}$$

The **boldface numerics** are multinomial coefficients: they answer the question "In how many distinct ways can the following E-factors be ordered?" The terms that enter into the construction of P_n arise—one for one—from the distinct partitions of n, and are $p(n)$ in number (which is to say: their number grows exponentially).

Each $\Pi_p(E^0)$ is (for $p > 0$) a *sum* of products. Some of the summed terms contain $(E_n^0 - E^0)$ as a factor, others don't. We formalize the distinction, writing

$$\begin{aligned} \Pi_0(E^0) &= A_1(E^0) \cdot (E_n^0 - E^0) \\ \Pi_1(E^0) &= A_2(E^0) \cdot (E_n^0 - E^0) + A_1(E^0) \\ \Pi_2(E^0) &= A_3(E^0) \cdot (E_n^0 - E^0) + A_2(E^0) \\ &\ \vdots \end{aligned} \tag{15}$$

The expressions $A_p(E^0)$ are constructed this way: strike p factors from P_0 in all possible ways; abandon the expressions that contain $(E_n^0 - E^0)$-factors; sum the terms that survive... but that is of little consequence: the coefficients A_p function in the present theory as *formal placeholders*; their *numerical* values are, for realistic unperturbed spectra, typically *infinite* (though certainly finite if $\mathbb{H}^0$ is finite-dimensional).

When (13) comes into play we will have

$$D \equiv D_{nn} \equiv (E_n^0 - E^0)\Big|_{E^0 \to E_n^0} = 0$$

but it is vital that we hold that fact in suspension, for soon we will encounter D^{-1}-factors, and our ultimate success hinges on our ability to write $D \cdot D^{-1} = 1$. Let (15) be abbreviated

$$\begin{aligned} \Pi_0 &= \phantom{A_1 +{}} DA_1 \\ \Pi_1 &= A_1 + DA_2 \\ \Pi_2 &= A_2 + DA_3 \\ &\vdots \end{aligned} \tag{16}$$

Returning with this information to (14) we obtain

$$\begin{aligned} P_0 &= \phantom{P_{10} +{}} DP_{01} \\ P_1 &= P_{10} + DP_{11} \\ P_2 &= P_{20} + DP_{21} \\ &\vdots \end{aligned} \tag{17}$$

where the leading index on refers to expansion in powers of λ, and the trailing index to expansion in reciprocal powers of D. To facilitate further progress, we make a

> NOTATIONAL ADJUSTMENT: Agree henceforth to write E_1 for E_n^1, E_2 for E_n^2, etc. and to interpret superscripts to mean true exponents: E_1^3 will mean $(E_n^1)^3$, etc. We will be thus released from the obligation of having to write expressions like $E_n^1 E_n^1 E_n^1$, which become unworkable in high order.

That understood, we introduce (16) into (14), and in the notation of (17) obtain

$$P_{01} = A_1 \tag{18.01}$$

$$P_{10} = -A_1 E_1 \tag{18.10}$$

$$P_{11} = -A_2 E_1 \tag{18.11}$$

$$P_{20} = -A_1 E_2 + A_2 E_1^2 \tag{18.20}$$

$$P_{21} = -A_2 E_2 + A_3 E_1^2 \tag{18.21}$$

$$P_{30} = -A_1 E_3 + 2A_2 E_1 E_2 - A_3 E_1^3 \tag{18.30}$$

$$P_{31} = -A_2 E_3 + 2A_3 E_1 E_2 - A_4 E_1^3 \tag{18.31}$$

$$P_{40} = -A_1 E_4 + A_2(E_2^2 + 2E_1 E_3) - 3A_3 E_1^2 E_2 + A_4 E_1^4 \tag{18.40}$$

$$P_{41} = -A_2 E_4 + A_3(E_2^2 + 2E_1 E_3) - 3A_4 E_1^2 E_2 + A_5 E_1^4 \tag{18.41}$$

$$\begin{aligned} P_{50} = -A_1 E_5 &+ A_2(2E_2 E_3 + 2E_1 E_4) \\ &- A_3(3E_1 E_2^2 + 3E_1^2 E_3) + 4A_4 E_1^3 E_2 - A_5 E_1^5 \end{aligned} \tag{18.50}$$

$$\begin{aligned} P_{51} = -A_2 E_5 &+ A_3(2E_2 E_3 + 2E_1 E_4) \\ &- A_4(3E_1 E_2^2 + 3E_1^2 E_3) + 4A_5 E_1^3 E_2 - A_6 E_1^5 \end{aligned} \tag{18.51}$$

Trace expansions. From

$$T_p \equiv \mathrm{tr}\,\mathbb{M}^p \quad \text{with} \quad \mathbb{M} \equiv \left\| \frac{V_{ij}}{E_i^0 - E} \right\|$$

we obtain

$$\begin{aligned} T_1(E) &= \sum_i \frac{V_{ii}}{E_i^0 - E} \\ T_2(E) &= \sum_{ij} \frac{V_{ij}V_{ji}}{(E_i^0 - E)(E_j^0 - E)} \\ T_3(E) &= \sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{(E_i^0 - E)(E_j^0 - E)(E_k^0 - E)} \\ &\vdots \end{aligned}$$

Therefore

$$\begin{aligned} T_1(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots) &= \sum_i \frac{V_{ii}}{E_i^0 - E_n^0}\Big[1 - \frac{\lambda E_n^1 + \lambda^2 E_n^2 + \cdots}{E_i^0 - E_n^0}\Big]^{-1} \\ &= \sum_i \frac{V_{ii}}{D_{in}}\big[\text{etc.}\big]_i^{-1} \qquad (19.1) \\ &\equiv T_{10} + \lambda T_{11} + \lambda^2 T_{12} + \cdots \end{aligned}$$

$$\begin{aligned} T_2(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots) &= \sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}}\big[\text{etc.}\big]_i^{-1}\big[\text{etc.}\big]_j^{-1}. \qquad (19.2) \\ &\equiv T_{20} + \lambda T_{21} + \lambda^2 T_{22} + \cdots \end{aligned}$$

$$\begin{aligned} T_3(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots) &= \sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{D_{in}D_{jn}D_{kn}}\big[\text{etc.}\big]_i^{-1}\big[\text{etc.}\big]_j^{-1}\big[\text{etc.}\big]_k^{-1} \qquad (19.3) \\ &\equiv T_{30} + \lambda T_{31} + \lambda^2 T_{32} + \cdots \\ &\vdots \end{aligned}$$

Entrusting the computational labor to *Mathematica* we obtain[3]

$$\begin{aligned} \big[\text{etc.}\big]_i^{-1} = 1 + \lambda\ &\Big[\tfrac{E_1}{D_{in}}\Big] \\ + \lambda^2&\Big[\tfrac{E_1^2}{D_{in}^2} + \tfrac{E_2}{D_{in}}\Big] \\ + \lambda^3&\Big[\tfrac{E_1^3}{D_{in}^3} + \tfrac{2E_1E_2}{D_{in}^2} + \tfrac{E_3}{D_{in}}\Big] \\ + \lambda^4&\Big[\tfrac{E_1^4}{D_{in}^4} + \tfrac{3E_1^2E_2}{D_{in}^3} + \tfrac{2E_1E_3 + E_2E_2}{D_{in}^2} + \tfrac{E_4}{D_{in}}\Big] \\ + \lambda^5&\Big[\tfrac{E_1^5}{D_{in}^5} + \tfrac{4E_1^3E^2}{D_{in}^4} + \tfrac{3E_1^2E_3 + 3E_1E_2^2}{D_{in}^3} \\ &\qquad + \tfrac{2E_1E_4 + 2E_2E_3}{D_{in}^2} + \tfrac{E_5}{D_{in}}\Big] + \cdots \qquad (20) \end{aligned}$$

[3] The numerical factors on the right side the following expression enter for the same partition-theoretic reason as was previously discussed.

which becomes rapidly quite unwieldly when raised to powers, as (11) requires. Expressions like $\big[\text{etc.}\big]_i^{-1}\big[\text{etc.}\big]_j^{-1}$, $\big[\text{etc.}\big]_i^{-1}\big[\text{etc.}\big]_j^{-1}\big[\text{etc.}\big]_k^{-1}$, ... are unwieldly for an identical reason.

Further complications—which turn out, however, to be the key to the success of the determinantal method!—arise from the circumstance that some of the energy denominators which enter into expressions like

$$\sum_i \frac{V_{ii}}{D_{in}}, \quad \sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}}, \quad \sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{D_{in}D_{jn}D_{kn}}, \ldots$$

vanish,[4] causing the expressions themselves to become singular. It is to expose the singularities that we write

$$\sum_i \frac{V_{ii}}{D_{in}} = \sum_{i\neq n} \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D} \tag{21.1}$$

$$\sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} = \sum_{ij\neq n} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_{j\neq n} \frac{V_{nj}V_{jn}}{DD_{jn}} + \frac{V_{nn}V_{nn}}{D^2} \tag{21.2}$$

$$\begin{aligned}\sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{D_{in}D_{jn}D_{kn}} = \sum_{ijk\neq n} \frac{V_{ij}V_{jk}V_{ki}}{D_{in}D_{jn}D_{kn}} &+ 3\sum_{jk\neq n} \frac{V_{nj}V_{jk}V_{kn}}{DD_{jn}D_{kn}} \\ &+ 3\sum_{k\neq n} \frac{V_{nn}\cdot V_{nk}V_{kn}}{D^2 D_{kn}} + \frac{V_{nn}V_{nn}V_{nn}}{D^3}\end{aligned} \tag{21.3}$$

$$\vdots$$

where the numerics are binomial coefficients.

Additional powers of D^{-1} are brought into play when expressions like (20) are introduced into the summands. To gain a sharpened sense of the particulars we use (21) and (20) to obtain

$$T_{10} = \sum_i \frac{V_{ii}}{D_{in}} 1 = \sum_{i\neq n} \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D} \tag{22.1}$$

$$T_{11} = \sum_i \frac{V_{ii}}{D_{in}} \left[\frac{E_1}{D_{in}}\right] = E_1\left\{\sum_{i\neq n} \frac{V_{ii}}{D_{in}^2} + \frac{V_{nn}}{D^2}\right\} \tag{22.2}$$

$$T_{20} = \sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} 1 = \sum_{ij\neq n} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_{j\neq n} \frac{V_{nj}V_{jn}}{DD_{jn}} + \frac{V_{nn}V_{nn}}{D^2} \tag{22.3}$$

which when brought to (11.1) and (11.2) inform us that

$$Q_1 = \boxed{\text{TERMS}}_{1,0} + \frac{1}{D}\boxed{\text{TERMS}}_{1,1}$$

$$Q_2 = \boxed{\text{TERMS}}_{2,0} + \frac{1}{D}\boxed{\text{TERMS}}_{2,1} + \frac{1}{D^2}\boxed{\text{TERMS}}_{2,2}$$

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[4] The assignment $E^0 \mapsto E_n^0$ sends $D_i \equiv (E_i^0 - E^0) \mapsto (E_i^0 - E_n^0) \equiv D_{in}$, which vanishes at $i = n$.

This line of argument leads to the conclusion that

$$\begin{aligned} Q_1 &= Q_{10} + D^{-1}Q_{11} \\ Q_2 &= Q_{20} + D^{-1}Q_{21} + D^{-2}Q_{22} \\ Q_3 &= Q_{30} + D^{-1}Q_{31} + D^{-2}Q_{32} + D^{-3}Q_{33} \\ &\vdots \end{aligned} \tag{23}$$

where—as also at (17)—the leading index on refers to expansion in powers of λ, and the trailing index to expansion in reciprocal powers of D.

Development of the double series

$$T_p \equiv \operatorname{tr} \mathbb{M}^p = \sum_i \lambda^i T_{pi} \tag{24.1}$$

$$T_{pi} = \sum_{q=0}^{p+i} T_{piq} D^{-q} \tag{24.2}$$

(which feeds—by (11)—into the design of the Q_{iq}) is tedious work. One of the fruits of the discussion to which I now turn will be a precise description of the *details which actually contribute* to perturbation theory in any specified order.

Distilled essence of the determinantal method. Return with (18) and (22) to (12) and with the assistance of *Mathematica* obtain

$$\begin{aligned} 0 &= \big[P_{10} + P_{01}Q_{11}\big] \\ &\qquad + D\big[P_{11} + P_{01}Q_{10}\big] \\ &\equiv \boxed{\text{GOOD STUFF}}_1 + D\,\boxed{\text{DOOMED STUFF}}_1 \end{aligned}$$

$$\begin{aligned} 0 &= \big[P_{20} + P_{10}Q_{10} + P_{11}Q_{11} + P_{01}Q_{21}\big] \\ &\qquad + D\big[P_{21} + P_{11}Q_{10} + P_{01}Q_{20}\big] \\ &\qquad + D^{-1}\big[P_{10}Q_{11} + P_{01}Q_{22}\big] \\ &\equiv \boxed{\text{GOOD STUFF}}_2 + D\,\boxed{\text{DOOMED STUFF}}_2 + D^{-1}\,\boxed{\text{NULL STUFF}}_{2,1} \end{aligned}$$

$$\begin{aligned} 0 &= \big[P_{30} + P_{20}Q_{10} + P_{21}Q_{11} + P_{10}Q_{20} + P_{11}Q_{21} + P_{01}Q_{31}\big] \\ &\qquad + D\big[P_{31} + P_{21}Q_{10} + P_{11}Q_{20} + P_{01}Q_{30}\big] \\ &\qquad + D^{-1}\big[P_{20}Q_{11} + P_{10}Q_{21} + P_{11}Q_{22} + P_{01}Q_{32}\big] \\ &\qquad + D^{-2}\big[P_{10}Q_{22} + P_{01}Q_{33}\big] \\ &\equiv \boxed{\text{GOOD STUFF}}_3 + D\,\boxed{\text{DOOMED STUFF}}_3 + D^{-1}\,\boxed{\text{NULL STUFF}}_{3,1} \\ &\qquad\qquad + D^{-2}\,\boxed{\text{NULL STUFF}}_{3,2} \end{aligned}$$

The $\boxed{\text{DOOMED STUFF}}$ is killed by the process $D \to 0$. In Part A I provide explicit demonstrations that

$$\boxed{\text{NULL STUFF}}_{2,1} = \boxed{\text{NULL STUFF}}_{3,1} = \boxed{\text{NULL STUFF}}_{3,2} = 0$$

hold unconditionally, as consequences simply of the detailed construction of those expressions. I do not know how to construct such arguments in the general case, but will proceed in confidence that

$$\boxed{\text{NULL STUFF}} = 0 \text{ in all cases} \tag{25}$$

since were it otherwise the right side of (4) would exhibit singularities which are manifestly absent from the left side.

"Determinantal perturbation theory," boiled down to its essence, resides therefore in the following sequential statements:

$$\left.\begin{aligned} \boxed{\text{GOOD STUFF}}_1 &= 0\\ \boxed{\text{GOOD STUFF}}_2 &= 0\\ \boxed{\text{GOOD STUFF}}_3 &= 0\\ \boxed{\text{GOOD STUFF}}_4 &= 0\\ \boxed{\text{GOOD STUFF}}_5 &= 0\\ &\vdots \end{aligned}\right\} \tag{26}$$

which can be looked upon as a sharpened version of (12). When using the method in order p we need concern ourselves with trace expansions (first in powers of λ, then in inverse powers of D) only to the extent necessitated by the definitions of $\boxed{\text{GOOD STUFF}}_k$: $k = 1, 2, \ldots, p$. For future reference I record here that

$$\boxed{\text{GOOD STUFF}}_1 = P_{10} + P_{01}Q_{11} \tag{27.1}$$

$$\boxed{\text{GOOD STUFF}}_2 = P_{20} + P_{10}Q_{10} + P_{11}Q_{11} + P_{01}Q_{21} \tag{27.2}$$

$$\begin{aligned}\boxed{\text{GOOD STUFF}}_3 = P_{30} &+ P_{20}Q_{10} + P_{21}Q_{11} + P_{10}Q_{20}\\ &+ P_{11}Q_{21} + P_{01}Q_{31}\end{aligned} \tag{27.3}$$

$$\begin{aligned}\boxed{\text{GOOD STUFF}}_4 = P_{40} &+ P_{30}Q_{10} + P_{31}Q_{11} + P_{20}Q_{20}\\ &+ P_{21}Q_{21} + P_{10}Q_{30} + P_{11}Q_{31} + P_{01}Q_{41}\end{aligned} \tag{27.4}$$

$$\begin{aligned}\boxed{\text{GOOD STUFF}}_5 = P_{50} &+ P_{40}Q_{10} + P_{41}Q_{11} + P_{30}Q_{20} + P_{31}Q_{21}\\ &+ P_{20}Q_{30} + P_{21}Q_{31} + P_{10}Q_{40} + P_{11}Q_{41} + P_{01}Q_{51}\end{aligned} \tag{27.5}$$

Notice that advancing from one order to the next always brings two more terms into play; by this measure, complexity grows (not exponentially but only) linearly.

Evidently we need to possess descriptions of

$$\begin{array}{cclccl} & P_{01} & & & & \\ P_{10} & & \text{and} & & Q_{11} & \text{to work in order } p = 1\\ & & & & & \\ & P_{01} & & & & \\ P_{10} & P_{11} & \text{and} & Q_{10} & Q_{11} & \text{to work in order } p = 2\\ P_{20} & & & & Q_{21} & \end{array}$$

$$\begin{array}{ll} & P_{01} \\ P_{10} & P_{11} \\ P_{20} & P_{21} \\ P_{30} & \end{array} \quad \text{and} \quad \begin{array}{ll} Q_{10} & Q_{11} \\ Q_{20} & Q_{21} \\ & Q_{31} \end{array} \quad \text{to work in order } p = 3$$

$$\begin{array}{ll} & P_{01} \\ P_{10} & P_{11} \\ P_{20} & P_{21} \\ P_{30} & P_{31} \\ P_{40} & \end{array} \quad \text{and} \quad \begin{array}{ll} Q_{10} & Q_{11} \\ Q_{20} & Q_{21} \\ Q_{30} & Q_{31} \\ & Q_{41} \end{array} \quad \text{to work in order } p = 4$$

$$\begin{array}{ll} & P_{01} \\ P_{10} & P_{11} \\ P_{20} & P_{21} \\ P_{30} & P_{31} \\ P_{40} & P_{41} \\ P_{50} & \end{array} \quad \text{and} \quad \begin{array}{ll} Q_{10} & Q_{11} \\ Q_{20} & Q_{21} \\ Q_{30} & Q_{31} \\ Q_{40} & Q_{41} \\ & Q_{51} \end{array} \quad \text{to work in order } p = 5$$

The requisite P-data were produced already at (18). Detailed Q-data have yet to be generated, but from (11) we know that the only T_{pi} of interest in that connection are

$$T_{10} \qquad \text{if we work in order } p = 1$$

$$\begin{array}{ll} T_{10} & T_{11} \\ T_{20} & \end{array} \qquad \text{if we work in order } p = 2$$

$$\begin{array}{lll} T_{10} & T_{11} & T_{12} \\ T_{20} & T_{21} & \\ T_{30} & & \end{array} \qquad \text{if we work in order } p = 3$$

$$\begin{array}{llll} T_{10} & T_{11} & T_{12} & T_{13} \\ T_{20} & T_{21} & T_{22} & \\ T_{30} & T_{31} & & \\ T_{40} & & & \end{array} \qquad \text{if we work in order } p = 4$$

$$\begin{array}{lllll} T_{10} & T_{11} & T_{12} & T_{13} & T_{14} \\ T_{20} & T_{21} & T_{22} & T_{23} & \\ T_{30} & T_{31} & T_{32} & & \\ T_{40} & T_{41} & & & \\ T_{50} & & & & \end{array} \qquad \text{if we work in order } p = 5 \tag{28}$$

And it is gratifying to note that, once those terms have been packaged as required by (11), their D^{-1}-expansion need be carried only to first order. One would, on the other hand, have to work in much more elaborate detail if one sought to construct *explicit demonstrations* of all statements of type (25); it is by abandoning that redundant exercise (which, however, provides valuable checks on the *accuracy* of our work) that we have brought high-order perturbation theory within the bounds of feasibility.

Truncated double expansion of trace terms. Here I undertake to construct equations of (compare (24)) the form

$$T_{pi} \approx T_{pi0} + T_{pi1}D^{-1} \tag{30}$$

where ${}_{pi}$ ranges on the values indicated at (26) and where $\approx$ signifies that terms of orders D^{-2}, D^{-3}, ... have been dismissed on the ground that *in the non-degenerage case* they have nothing to tell us, are irrelevant to determinantal perturbation theory (though of vital relevance to the verification of (25)). Our (labor-intensive) computational program was anticipated at (22), where we obtained results which—if, to reduce notational clutter, we adopt a "summation convention" according to which

$$\sum_{i\neq n}, \quad \sum_{ij\neq n}, \quad \sum_{ijk\neq n}, \quad \ldots \text{ will be tacitly understood}$$

—can be expressed

$$\begin{aligned} T_{10} &\approx \frac{V_{ii}}{D_{in}} + V_{nn}D^{-1} \\ T_{11} &\approx E_1\frac{V_{ii}}{D_{in}^2} \\ T_{20} &\approx \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\frac{V_{nj}V_{jn}}{D_{jn}}D^{-1} \end{aligned}$$

Proceding similarly with the indispensable assistance of *Mathematica*, I construct this extension of the preceding short list:

$$T_{10} \approx \left\{\frac{1}{D_{in}}\right\}V_{ii} + V_{nn}D^{-1} \tag{31.10}$$

$$T_{11} \approx \left\{E_1\frac{1}{D_{in}^2}\right\}V_{ii} \tag{31.11}$$

$$T_{12} \approx \left\{E_1^2\frac{1}{D_{in}^3} + E_2\frac{1}{D_{in}^2}\right\}V_{ii} \tag{31.12}$$

$$T_{13} \approx \left\{E_1^3\frac{1}{D_{in}^4} + 2E_1E_2\frac{1}{D_{in}^3} + E_3\frac{1}{D_{in}^2}\right\}V_{ii} \tag{31.13}$$

$$T_{14} \approx \left\{E_1^4\frac{1}{D_{in}^5} + 3E_1^2E_2\frac{1}{D_{in}^4} + (2E_1E_3 + E_2^2)\frac{1}{D_{in}^3} + E_4\frac{1}{D_{in}^2}\right\}V_{ii} \tag{31.14}$$

$$T_{20} \approx \left\{\frac{1}{D_{in}D_{jn}}\right\}V_{ij}V_{ji} + 2\left\{\frac{1}{D_{jn}}\right\}V_{nj}V_{jn}D^{-1} \tag{31.20}$$

$$T_{21} \approx \left\{E_1\left[\frac{1}{D_{in}D_{jn}^2} + \frac{1}{D_{in}^2D_{jn}}\right]\right\}V_{ij}V_{ji} + 2\left\{E_1\frac{1}{D_{jn}^2}\right\}V_{nj}V_{jn}D^{-1} \tag{31.21}$$

$$T_{22} \approx \Big\{E_1^2\Big[\frac{1}{D_{in}D_{jn}^3} + \frac{1}{D_{in}^2D_{jn}^2} + \frac{1}{D_{in}^3D_{jn}}\Big] \tag{31.22}$$
$$+ E_2\Big[\frac{1}{D_{in}D_{jn}^2} + \frac{1}{D_{in}^2D_{jn}}\Big]\Big\}V_{ij}V_{ji}$$
$$+ 2\Big\{E_1^2\frac{1}{D_{jn}^3} + E_2\frac{1}{D_{jn}^2}\Big\}V_{nj}V_{jn}D^{-1}$$

$$T_{23} \approx \Big\{E_1^3\Big[\frac{1}{D_{in}D_{jn}^4} + \frac{1}{D_{in}^2D_{jn}^3} + \frac{1}{D_{in}^3D_{jn}^2} + \frac{1}{D_{in}^4D_{jn}}\Big] \tag{31.23}$$
$$+ 2E_1E_2\Big[\frac{1}{D_{in}D_{jn}^3} + \frac{1}{D_{in}^2D_{jn}^2} + \frac{1}{D_{in}^3D_{jn}}\Big]$$
$$+ E_3\Big[\frac{1}{D_{in}D_{jn}^2} + \frac{1}{D_{in}^2D_{jn}}\Big]\Big\}V_{ij}V_{ji}$$
$$+ 2\Big\{E_1^3\frac{1}{D_{jn}^4} + 2E_1E_2\frac{1}{D_{jn}^3} + E_3\frac{1}{D_{jn}^2}\Big\}V_{nj}V_{jn}D^{-1}$$

$$T_{30} \approx \Big\{\frac{1}{D_{in}D_{jn}D_{kn}}\Big\}V_{ij}V_{jk}V_{ki} + 3\Big\{\frac{1}{D_{jn}D_{kn}}\Big\}V_{nj}V_{jk}V_{kn}D^{-1} \tag{31.30}$$

$$T_{31} \approx \Big\{E_1\Big[\frac{1}{D_{in}^2D_{jn}D_{kn}} + \frac{1}{D_{in}D_{jn}^2D_{kn}} + \frac{1}{D_{in}D_{jn}D_{kn}^2}\Big]\Big\}V_{ij}V_{jk}V_{ki}$$
$$+ 3\Big\{E_1\Big[\frac{1}{D_{jn}^2D_{kn}} + \frac{1}{D_{jn}D_{kn}^2}\Big]\Big\}V_{nj}V_{jk}V_{kn}D^{-1} \tag{31.31}$$

$$T_{32} \approx \Big\{E_1^2\Big[\frac{1}{D_{in}^3D_{jn}D_{kn}} + \frac{1}{D_{in}D_{jn}^3D_{kn}} + \frac{1}{D_{in}D_{jn}D_{kn}^3} \tag{31.32}$$
$$+ \frac{1}{D_{in}D_{jn}^2D_{kn}^2} + \frac{1}{D_{in}^2D_{jn}D_{kn}^2} + \frac{1}{D_{in}^2D_{jn}^2D_{kn}}\Big]$$
$$+ E_2\Big[\frac{1}{D_{in}^2D_{jn}D_{kn}} + \frac{1}{D_{in}D_{jn}^2D_{kn}} + \frac{1}{D_{in}D_{jn}D_{kn}^2}\Big]\Big\}V_{ij}V_{jk}V_{ki}$$
$$+ 3\Big\{E_1^2\Big[\frac{1}{D_{jn}^3D_{kn}} + \frac{1}{D_{jn}D_{kn}^3} + \frac{1}{D_{jn}^2D_{kn}^2}\Big]$$
$$+ E_2\Big[\frac{1}{D_{jn}^2D_{kn}} + \frac{1}{D_{jn}D_{kn}^2}\Big]\Big\}V_{nj}V_{jk}V_{kn}D^{-1}$$

$$T_{40} \approx \Big\{\frac{1}{D_{in}D_{jn}D_{kn}D_{ln}}\Big\}V_{ij}V_{jk}V_{kl}V_{li} \tag{31.40}$$
$$+ 4\Big\{\frac{1}{D_{jn}D_{kn}D_{ln}}\Big\}V_{nj}V_{jk}V_{kl}V_{ln}D^{-1}$$

$$T_{41} \approx \Big\{E_1\Big[\frac{1}{D_{in}^2 D_{jn} D_{kn} D_{ln}} + \frac{1}{D_{in} D_{jn}^2 D_{kn} D_{ln}} + \frac{1}{D_{in} D_{jn} D_{kn}^2 D_{ln}} + \frac{1}{D_{in} D_{jn} D_{kn} D_{ln}^2}\Big]\Big\} V_{ij}V_{jk}V_{kl}V_{li} + 4\Big\{E_1\Big[\frac{1}{D_{jn}^2 D_{kn} D_{ln}} + \frac{1}{D_{jn} D_{kn}^2 D_{ln}} + \frac{1}{D_{jn} D_{kn} D_{ln}^2}\Big]\Big\} V_{nj}V_{jk}V_{kl}V_{ln}D^{-1} \tag{31.41}$$

$$T_{50} \approx \frac{1}{D_{in}D_{jn}D_{kn}D_{ln}D_{mn}} V_{ij}V_{jk}V_{kl}V_{lm}V_{mi} + 5\frac{1}{D_{jn}D_{kn}D_{ln}D_{mn}} V_{nj}V_{jk}V_{kl}V_{lm}V_{mn}D^{-1} \tag{31.50}$$

We note—as a weak check on the accuracy of those statements—that every term is physically dimensionless.

Equations (11) ask us to *multiply* the T_{pi} in various ways... and this, unless we are careful, can lead to deep confusion. Look, for example, to the product $T_{10}^2 T_{11}$ encountered in (11.4): were we to proceed literally from (31.10) and (31.11) we—*Mathematica*—would obtain

$$T_{10}^2 T_{11} \approx E_1 \frac{V_{ii}^3}{D_{in}^4} + 2E_1 \frac{V_{ii}^2 V_{nn}}{D_{in}^3} D^{-1}$$

which is incorrect: we have displayed as a sum of products what is really a product of sums—this because we have not distinguished the running index in one sum from the running index in the other. And we would soon run out of alphabet if we attempted (by hand) to maintain the indicial distinctions in question. I propose, therefore, to give each sum its own distinctive name: I will write

$$T_{10} \approx \Sigma_{10} + \sigma_{10}D^{-1} \tag{32.10}$$

$$T_{11} \approx E_1\Sigma_{11} \tag{32.11}$$

$$T_{12} \approx E_1^2\Sigma_{12} + E_2\Sigma_{11} \tag{32.12}$$

$$T_{13} \approx E_1^3\Sigma_{13} + 2E_1E_2\Sigma_{12} + E_3\Sigma_{11} \tag{32.13}$$

$$T_{14} \approx E_1^4\Sigma_{14} + 3E_1^2E_2\Sigma_{13} + (2E_1E_3 + E_2^2)\Sigma_{12} + E_4\Sigma_{11} \tag{32.14}$$

$$T_{20} \approx \Sigma_{20} + \sigma_{20}D^{-1} \tag{32.20}$$

$$T_{21} \approx E_1\Sigma_{21} + E_1\sigma_{21}D^{-1} \tag{32.21}$$

$$T_{22} \approx E_1^2\Sigma_{22} + E_2\Sigma_{21} + \big\{E_1^2\sigma_{22} + E_2\sigma_{21}\big\}D^{-1} \tag{32.22}$$

$$T_{23} \approx E_1^3\Sigma_{23} + 2E_1E_2\Sigma_{22} + E_3\Sigma_{21} + \big\{E_1^3\sigma_{23} + 2E_1E_2\sigma_{22} + E_3\sigma_{21}\big\}D^{-1} \tag{32.23}$$

$$T_{30} \approx \Sigma_{30} + \sigma_{30} D^{-1} \tag{32.30}$$
$$T_{31} \approx E_1\Sigma_{31} + E_1\sigma_{31} D^{-1} \tag{32.31}$$
$$T_{32} \approx E_1^2\Sigma_{32} + E_2\Sigma_{31} + \big\{E_1^2\sigma_{32} + E_2\sigma_{31}\big\} D^{-1} \tag{32.32}$$
$$T_{40} \approx \Sigma_{40} + \sigma_{40} D^{-1} \tag{32.40}$$
$$T_{41} \approx E_1\Sigma_{41} + E_1\sigma_{41} D^{-1} \tag{32.41}$$
$$T_{50} \approx \Sigma_{50} + \sigma_{50} D^{-1} \tag{32.50}$$

and look to (31) for the *definitions* of the Σ's and σ's, which are, in effect, "encapsulated sums." Equations (32) show (31) to have been more highly patterned than you may at first have noticed, and from the precision of that pattern we gain confidence in the accuracy of (31/32).

Construction of the truncated Q-coefficients. We introduce (32) into (11), expand in powers of D^{-1}, abandon the terms of orders D^{-2}, D^{-3}, . . . and, consigning all the labor to *Mathematica*, obtain

$$Q_{10} \approx \Sigma_{10} \tag{33.10}$$
$$Q_{11} \approx \sigma_{10} \tag{33.11}$$
$$Q_{20} \approx E_1\Sigma_{11} + \tfrac{1}{2}\big[\Sigma_{10}^2 - \Sigma_{20}\big] \tag{33.20}$$
$$Q_{21} \approx \sigma_{10}\Sigma_{10} - \tfrac{1}{2}\sigma_{20} \tag{33.21}$$
$$Q_{30} \approx E_1^2\Sigma_{12} + E_1\big[\Sigma_{10}\Sigma_{11} - \tfrac{1}{2}\Sigma_{21}\big] + E_2\Sigma_{11} + \big[\tfrac{1}{6}\Sigma_{10}^3 - \tfrac{1}{2}\Sigma_{10}\Sigma_{20} + \tfrac{1}{3}\Sigma_{30}\big] \tag{33.30}$$
$$Q_{31} \approx E_1\big[\sigma_{10}\Sigma_{11} - \tfrac{1}{2}\sigma_{21}\big] + \big[\tfrac{1}{3}\sigma_{30} + \tfrac{1}{2}(\sigma_{10}\Sigma_{10}^2 - \sigma_{20}\Sigma_{10} - \sigma_{10}\Sigma_{20})\big] \tag{33.31}$$

The descriptions of

$$Q_{40} \approx \text{sum of 17 terms}$$
$$Q_{41} \approx \text{sum of 16 terms}$$
$$Q_{50} \approx \text{sum of 37 terms}$$
$$Q_{51} \approx \text{sum of 41 terms}$$

are so uninformatively complicated that they will be reserved for an appendix.

Final assembly. Bring the $Q_{\bullet\bullet}$ of (33) and the $P_{\bullet\bullet}$ of (18) to (27), and obtain

$$\boxed{\text{GOOD STUFF}}_1 = -A_1\big\{E_1 - \sigma_{10}\big\}$$
$$\boxed{\text{GOOD STUFF}}_2 = \big(A_2E_1 - A_1\Sigma_{10}\big)\big\{E_1 - \sigma_{10}\big\} - A_1\big\{E_2 + \tfrac{1}{2}\sigma_{20}\big\}$$
$$\begin{aligned}\boxed{\text{GOOD STUFF}}_3 = \tfrac{1}{2}\big(&- A_3E_1^2 - A_2(\sigma_{20} - 2E_1\Sigma_{10}) \\ &- A_1(\sigma_{21} + \Sigma_{10}^2 + 2E_1\Sigma_{11} - \Sigma_{10})\big)\big\{E_1 - \sigma_{10}\big\} \\ &+ \tfrac{1}{4}\big(A_2(2E_2 - \sigma_{10}) - A_1\Sigma_{10}\big)\big\{E_2 + \tfrac{1}{2}\sigma_{20}\big\} \\ &- A_1\big\{E_3 + \tfrac{1}{2}\sigma_{10}\sigma_{21} - \tfrac{1}{3}\sigma_{30}\big\}\end{aligned}$$

The detail is distracting; the *Mathematica* commands themselves seem in this instance to be more instructive: ask for `good1` and get

$$-A_1\big(E_1-\sigma_{10}\big)$$

Enter the command `Simplify[good2,` $\mathtt{E}_1-\sigma_{10}==0$`]` and get

$$-A_1\big(E_2+\tfrac{1}{2}\sigma_{20}\big)$$

Command `Simplify[good3,` $\{\mathtt{E}_1-\sigma_{10}==0, \mathtt{E}_2+\tfrac{1}{2}\sigma_{20}==0\}$`]` and get

$$-A_1\big(E_3+\tfrac{1}{2}\sigma_{10}\sigma_{21}-\tfrac{1}{3}\sigma_{30}\big)$$

The next two generations of this sequential procedure give

$$-A_1\big(E_4-\tfrac{1}{4}\sigma_{20}\sigma_{21}+\tfrac{1}{2}E_1^2\sigma_{22}-\tfrac{1}{3}E_1\sigma_{31}+\tfrac{1}{4}\sigma_{40}\big),$$

$$\begin{aligned}-A_1\big(E_5+\tfrac{1}{2}E_3\sigma_{21}+E_2\sigma_{10}\sigma_{22}+\tfrac{1}{2}\sigma_{10}^3\sigma_{23}-\tfrac{1}{3}E_2\sigma_{31}-\tfrac{1}{3}\sigma_{10}^2\sigma_{32}\\+\tfrac{1}{4}\sigma_{10}\sigma_{41}-\tfrac{1}{5}\sigma_{50}+\tfrac{1}{4}\sigma_{40}\Sigma_{10}+\tfrac{1}{4}\sigma_{10}\Sigma_{40}\big)\end{aligned}$$

The assumed non-degeneracy of E_n^0 implies $A_1\neq 0$, so on the basis of (26) we have[5]

$$E_n^1=\sigma_{10} \tag{34.1}$$

$$E_n^2=-\tfrac{1}{2}\sigma_{20} \tag{34.2}$$

$$E_n^3=-\tfrac{1}{2}\sigma_{10}\sigma_{21}+\tfrac{1}{3}\sigma_{30} \tag{34.3}$$

$$E_n^4=+\tfrac{1}{4}\sigma_{20}\sigma_{21}-\tfrac{1}{2}(E_1)^2\sigma_{22}+\tfrac{1}{3}E_1\sigma_{31}-\tfrac{1}{4}\sigma_{40} \tag{34.4}$$

$$\begin{aligned}E_n^5=-\tfrac{1}{2}E_3\sigma_{21}-E_2\sigma_{10}\sigma_{22}-\tfrac{1}{2}\sigma_{10}^3\sigma_{23}+\tfrac{1}{3}E_2\sigma_{31}+\tfrac{1}{3}\sigma_{10}^2\sigma_{32}\\-\tfrac{1}{4}\sigma_{10}\sigma_{41}+\tfrac{1}{5}\sigma_{50}-\tfrac{1}{4}\sigma_{40}\Sigma_{10}-\tfrac{1}{4}\sigma_{10}\Sigma_{40}\end{aligned} \tag{34.5}$$

Comparison of (32) with (31) provides these definitions:

$$\begin{aligned}&\sigma_{10}\equiv V_{nn}\\&\sigma_{20}\equiv 2\Big\{\frac{1}{D_{jn}}\Big\}V_{nj}V_{jn}\quad;\quad\sigma_{21}\equiv 2\Big\{\frac{1}{D_{jn}^2}\Big\}V_{nj}V_{jn}\\&\sigma_{30}\equiv 3\Big\{\frac{1}{D_{jn}D_{kn}}\Big\}V_{nj}V_{jk}V_{kn}\end{aligned}$$

So the first three of equations (34), when translated into orthodox notation, read

$$E_n^1=V_{nn} \tag{35.1}$$

$$E_n^2=-\sum_{j\neq n}\frac{V_{nj}V_{jn}}{D_{jn}} \tag{35.2}$$

$$E_n^3=\sum_{jk\neq n}\frac{V_{nj}V_{jk}V_{kn}}{D_{jn}D_{kn}}-V_{nn}\cdot\sum_{j\neq n}\frac{V_{nj}V_{jn}}{D_{jn}^2} \tag{35.3}$$

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[5] The right sides of (34) are written precisely as *Mathematica* produced them, but on the left I have reinstated $E_p\mapsto E_n^p$ where p refers to *perturbational order*—not to a power. But E_1^2 on the right side of (34.4) *is* a power.

These are precisely the results reported at (2): the first two equations can be found in any introductory quantum text,[6] while—as reported earlier—(35.3) can be found on page 136 of Landau & Lifshitz' 3rd revised edition (1977). An alternative formulation of the same result appears at (25.12) in Hans Bethe & Edwin Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (1957).

Extending our σ-list

$$\begin{aligned}\sigma_{22} &\equiv 2\frac{1}{D_{jn}^3}V_{nj}V_{jn}\\ \sigma_{31} &\equiv 3\Big[\frac{1}{D_{jn}^2 D_{kn}}+\frac{1}{D_{jn}D_{kn}^2}\Big]V_{nj}V_{jk}V_{kn}\\ \sigma_{40} &\equiv 4\frac{1}{D_{jn}D_{kn}D_{ln}}V_{nj}V_{jk}V_{kl}V_{ln}\end{aligned}$$

we find that in 4th order

$$\begin{aligned}E_n^4 = \Big[\sum_{i\neq n}\frac{1}{D_{in}}V_{ni}V_{in}\Big]\Big[\sum_{j\neq n}\frac{1}{D_{jn}^2}V_{nj}V_{jn}\Big] &- V_{nn}^2\sum_{i\neq n}\frac{1}{D_{jn}^3}V_{nj}V_{jn}\\ &+ V_{nn}\cdot\sum_{ij\neq n}\Big[\frac{1}{D_{in}^2 D_{jn}}+\frac{1}{D_{in}D_{jn}^2}\Big]V_{ni}V_{ij}V_{jn} \\ &- \sum_{ijk\neq n}\frac{1}{D_{in}D_{jn}D_{kn}}V_{ni}V_{ij}V_{jk}V_{kn}\end{aligned}\tag{35.4}$$

$$E_n^5 = \begin{cases}\text{expression based on (34.5) which could be}\\ \text{spelled out in similarly orthodox detail...}\end{cases}\tag{35.5}$$

...but I won't. My confidence in the accuracy of (34/35) is high, yet not so high but what I would have interest in the results achieved by someone with the patience to retrace my steps. I would be particularly interested in verification of my claim (at (34.5)) that Σ-terms make their first appearance in 5th order.

E-factors appear on the right sides of (34.4) and (34.5). Replace those with their upstream sigma-equivalents, then count terms. Find

1	term	in 1st order
1	term	in 2nd order
2	terms	in 3rd order
4	terms	in 4th order
10	terms	in 5th order

We would, on this weak evidence, not be surprised to encounter ~ 20 terms in 6th order.

[6] See, for example, the boxed equations (6.9) and (6.14) in David Griffiths' *Introduction to Quantum Mechanics* (1994).

Discussion. “Perturbed Spectra without $\overset{\text{it says here}}{\wedge}$ Pain” (Part A) was essentially a notebook—a record of my activity as, for the first time, I explored an idea that had come to mind during the writing of Chapter One of my Advanced Quantum Topics (2000).[7] My effort here has been to demonstrate how the technique developed there can be used to generate results of higher perturbative order. To that end, I have been—necessarily—at pains to expose more clearly the algorithmic essentials of the method. I have, for obvious expository reasons, set details down upon the page. . . but the point that has impressed me most strongly is that in practical application of the method one *need not* concern oneself with those details; one can allow them to float unseen in the mind of *Mathematica*.

If E_n^0 is *degenerate* then the placeholders A_i introduced at (15) acquire D-factors, with consequences that ripple downstream but which remain entirely susceptible to algorithmic description along the same basic lines. I have sketched how this works in Part A, but have elected not to pursue the topic here; I hope to construct a detailed account of “determinantal perturbation theory of degenerate spectra” on another occasion. . . or better: to persuade a student to do so!

Acknowledgements. This work has required very nearly the full limit of my patience. David Griffiths was good enough to read Part A very closely and critically, and I have been sustained by his expressed interest in the work. And I am indebted to Oz Bonfim for inspiring me to revisit to this topic, so far removed from my normal spheres of activity.

[7] On page 40 I record my “regret that I must, on this occasion, leave further details to the delight of the curious reader.”

Truncated Q-coefficients of higher order. Here I make good my promise to extend to 4[th] and 5[th] orders the results listed at (33)...though the exercise serves no constructive purpose: such information need not be brought into the light of day, is best allowed to remain within *Mathematica*'s silicon mind. I have made no attempt to organize the terms, but present them in the sequence selected by *Mathematica*.

$$
\begin{aligned}
Q_{40} = {} & \tfrac{1}{24}\Sigma_{10}^4 + E_3\Sigma_{11} + E_2\Sigma_{10}\Sigma_{11} + \tfrac{1}{2}E_1\Sigma_{10}^2\Sigma_{11} + \tfrac{1}{2}E_1^2\Sigma_{11}^2 + E_1E_2\Sigma_{12} \\
& + E_1^2\Sigma_{10}\Sigma_{12} + E_1^3\Sigma_{13} - \tfrac{1}{4}\Sigma_{10}^2\Sigma_{20} - \tfrac{1}{2}E_1\Sigma_{11}\Sigma_{20} + \tfrac{1}{8}\Sigma_{20}^2 - \tfrac{1}{2}E_2\Sigma_{21} \\
& - \tfrac{1}{2}E_1\Sigma_{10}\Sigma_{21} - \tfrac{1}{2}E_1^2\Sigma_{22} + \tfrac{1}{3}\Sigma_{10}\Sigma_{30} + \tfrac{1}{3}E_1\Sigma_{31} - \tfrac{1}{4}\Sigma_{40} \\
Q_{41} = {} & -\tfrac{1}{2}E_2\sigma_{21} - \tfrac{1}{2}E_1^2\sigma_{22} + \tfrac{1}{3}E_1\sigma_{31} - \tfrac{1}{4}\sigma_{40} - \tfrac{1}{2}E_1\sigma_{21}\Sigma_{10} + \tfrac{1}{3}\sigma_{30}\Sigma_{10} \\
& - \tfrac{1}{4}\sigma_{20}\Sigma_{10}^2 + \tfrac{1}{6}\sigma_{10}\Sigma_{10}^3 + E_2\sigma_{10}\Sigma_{11} - \tfrac{1}{2}E_1\sigma_{20}\Sigma_{11} + E_1\sigma_{10}\Sigma_{10}\Sigma_{11} \\
& + E_1^2\sigma_{10}\Sigma_{12} + \tfrac{1}{4}\sigma_{20}\Sigma_{20} - \tfrac{1}{2}\sigma_{10}\Sigma_{10}\Sigma_{20} - \tfrac{1}{2}E_1\sigma_{10}\Sigma_{21} + \tfrac{1}{3}\sigma_{10}\Sigma_{30} \\
Q_{50} = {} & \tfrac{1}{120}\Sigma_{10}^5 + E_4\Sigma_{11} + E_3\Sigma_{10}\Sigma_{11} + \tfrac{1}{2}E_2\Sigma_{10}^2\Sigma_{11} + \tfrac{1}{6}E_1\Sigma_{10}^3\Sigma_{11} + E_1E_2\Sigma_{11}^2 \\
& + \tfrac{1}{2}E_1^2\Sigma_{10}\Sigma_{11}^2 + E_2^2\Sigma_{12} + 2E_1E_3\Sigma_{12} + E_1E_2\Sigma_{10}\Sigma_{12} + \tfrac{1}{2}E_1^2\Sigma_{10}^2\Sigma_{12} \\
& + E_1^3\Sigma_{11}\Sigma_{12} + 3E_1^2E_2\Sigma_{13} + E_1^3\Sigma_{10}\Sigma_{13} + E_1^4\Sigma_{14} - \tfrac{1}{12}\Sigma_{10}^3\Sigma_{20} \\
& - \tfrac{1}{2}E_2\Sigma_{11}\Sigma_{20} - \tfrac{1}{2}E_1\Sigma_{10}\Sigma_{11}\Sigma_{20} - \tfrac{1}{2}E_1^2\Sigma_{12}\Sigma_{20} + \tfrac{1}{8}\Sigma_{10}\Sigma_{20}^2 - \tfrac{1}{2}E_3\Sigma_{21} \\
& - \tfrac{1}{2}E_2\Sigma_{10}\Sigma_{21} - \tfrac{1}{4}E_1\Sigma_{10}^2\Sigma_{21} - \tfrac{1}{2}E_1^2\Sigma_{11}\Sigma_{21} + \tfrac{1}{4}E_1\Sigma_{20}\Sigma_{21} \\
& - E_1E_2\Sigma_{22} - \tfrac{1}{2}E_1^2\Sigma_{10}\Sigma_{22} - \tfrac{1}{2}E_1^3\Sigma_{23} + \tfrac{1}{6}\Sigma_{10}^2\Sigma_{30} + \tfrac{1}{3}E_1\Sigma_{11}\Sigma_{30} \\
& - \tfrac{1}{6}\Sigma_{20}\Sigma_{30} + \tfrac{1}{3}E_2\Sigma_{31} + \tfrac{1}{3}E_1\Sigma_{10}\Sigma_{31} + \tfrac{1}{3}E_1^2\Sigma_{32} - \tfrac{1}{2}\Sigma_{10}\Sigma_{40} \\
& - \tfrac{1}{4}E_1\Sigma_{41} + \tfrac{1}{5}\Sigma_{50} \\
Q_{51} = {} & -\tfrac{1}{2}E_3\sigma_{21} - E_1E_2\sigma_{22} - \tfrac{1}{2}E_1^3\sigma_{23} + \tfrac{1}{3}E_2\sigma_{31} + \tfrac{1}{3}E_1^2\sigma_{32} - \tfrac{1}{4}E_1\sigma_{41} + \tfrac{1}{5}\sigma_{50} \\
& - \tfrac{1}{2}E_2\sigma_{21}\Sigma_{10} - \tfrac{1}{2}E_1^2\sigma_{22}\Sigma_{10} + \tfrac{1}{3}E_1\sigma_{31}\Sigma_{10} - \tfrac{1}{2}\sigma_{40}\Sigma_{10} - \tfrac{1}{4}E_1\sigma_{21}\Sigma_{10}^2 \\
& + \tfrac{1}{6}\sigma_{30}\Sigma_{10}^2 - \tfrac{1}{12}\sigma_{20}\Sigma_{10}^3 + \tfrac{1}{24}\sigma_{10}\Sigma_{10}^4 + E_3\sigma_{10}\Sigma_{11} - \tfrac{1}{2}E_2\sigma_{20}\Sigma_{11} \\
& - \tfrac{1}{2}E_1^2\sigma_{21}\Sigma_{11} + \tfrac{1}{3}E_1\sigma_{30}\Sigma_{11} + E_2\sigma_{10}\Sigma_{10}\Sigma_{11} - \tfrac{1}{2}E_1\sigma_{20}\Sigma_{10}\Sigma_{11} \\
& + \tfrac{1}{2}E_1\sigma_{10}\Sigma_{10}^2\Sigma_{11} + \tfrac{1}{2}E_1^2\sigma_{10}\Sigma_{11}^2 + E_1E_2\sigma_{10}\Sigma_{12} - \tfrac{1}{2}E_1^2\sigma_{20}\Sigma_{12} \\
& + E_1^2\sigma_{10}\Sigma_{10}\Sigma_{12} + E_1^3\sigma_{10}\Sigma_{13} + \tfrac{1}{4}E_1\sigma_{21}\Sigma_{20} - \tfrac{1}{6}\sigma_{30}\Sigma_{20} \\
& + \tfrac{1}{4}\Sigma_{20}\Sigma_{10}\Sigma_{20} - \tfrac{1}{4}\sigma_{10}\Sigma_{10}^2\Sigma_{20} - \tfrac{1}{2}E_1\sigma_{10}\Sigma_{11}\Sigma_{20} + \tfrac{1}{8}\sigma_{10}\Sigma_{20}^2 \\
& - \tfrac{1}{2}E_2\sigma_{10}\Sigma_{21} + \tfrac{1}{4}E_1\sigma_{20}\Sigma_{21} - \tfrac{1}{2}E_1\sigma_{10}\Sigma_{10}\Sigma_{21} - \tfrac{1}{2}E_1^2\sigma_{10}\Sigma_{22} \\
& - \tfrac{1}{6}\sigma_{20}\Sigma_{30} + \tfrac{1}{3}\sigma_{10}\Sigma_{10}\Sigma_{30} + \tfrac{1}{3}E_1\sigma_{10}\Sigma_{11} - \tfrac{1}{2}\sigma_{10}\Sigma_{40}
\end{aligned}
$$

Such are the terms which *Mathematica* has been happy to multiply together and combine in a great variety of ways to achieve final results which we now recognize to be *astounding in their simplicity*!

"Determinantal spectral perturbation theory" provides what is from a mathematical viewpoint an *elementary exercise in formal series manipulation*, capable in principal of being extended to any order, but computationally so dense that its practical cultivation was virtually unthinkable prior to about 23 June 1988, when the first version of *Mathematica* was released.