it says here **PERTURBED SPECTRA WITHOUT** \land **PAIN**

New approach to time-independent perturbation theory

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Introduction. The term "spectrum" was introduced by Isaac Newton, who (later Master of the Mint) coined it to describe the colored lights which his prism had shown to be latently present—like ghostly spectres—in white light. The term radiated metaphorically throughout the language, but the usage that will concern us today is an apple that fell not far from the tree.

Quantum theory began as theory of thermalized light. It became quantum *mechanics* when Bohr (1913) described the Bohr atom, a mechanical structure intended to account for the hydrogen spectrum and, by extension, to lay the foundation for a general theory of atomic and molecular spectra. Bohr's striking success simulated theorists to play variations on Bohr's theme, in an effort to explain the small spectral adjustments which were observed to take place when atoms are subjected to various perturbations (Stark effect, Zeeman effect), and to account for certain subtlies evident in the spectroscopic data (spectral line shape).

A dozen years separate the work of Planck from that of Bohr. By the end of a second dozen years it had become evident to Heisenberg (who was twenty-four in 1925) that the characteristic energies $E_n = h\nu_n$ of atoms can be identified with characteristic numbers sequestered in the design of certain multi-component objects which Born recognized to be "matrices." Schrödinger, in 1926, published under the title "Quantization as an eigenvalue problem" a series of four papers¹ which took as their analytical method not matrix theory but the theory of differential equations (Sturm-Liouville theory), but it was clear to Schrödinger—and demonstrated in a paper which he inserted between Parts II & III of his main series—that "matrix mechanics" and "wave mechanics" are the same guy in different costumes. We are therefore not surprised, when we

¹ English translations of those and other classic papers have been reprinted in E. Schrödinger, *Collected Papers on Wave Mechanics* (1982).

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look back at the historical record, to discover that in his "Part III: Perturbation theory, with application to the Stark effect of the Balmer series"—where he describes the "time-independent perturbation theory" which has been reproduced in a thousand textbooks—Schrödinger adopts a distinctly matrix-theoretic mode of expression.

The time-independent Schrödinger equation, written in the abstracted notation devised by Dirac to achieve unification of the Heisenberg/Schrödinger theories, reads

$$\mathbf{H}|\psi) = E|\psi) \tag{1.1}$$

and with respect to any specified basis $\{|n\}$ acquires the representation

$$\sum (m|\mathbf{H}|n)(n|\psi) = (m|\psi) \quad \text{abbreviated} \quad \mathbb{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$$
(1.2)

This coupled system of linear equations admits of non-trivial solution if and only if E is a root of the characteristic polynomial

$$\det(\mathbb{H} - E\mathbb{I}) = 0 \tag{2}$$

The theory constructed by Schrödinger is a fully articulated creation that permits one to pose and attack a rich variety of ancillary questions, so we must look upon (2) as but an isolated detail within a theoretical tapestry. But in that detail Schrödinger made good his promise to present "quantization as an eigenvalue problem." Left in the dust—perceptible now only in blurred outline—is Bohr's original image of quantum mechanics as "classical mechanics adorned with an \hbar -dependent principle of orbital inclusion/exclusion," an image which had inspired a decade of work, but to which Heisenberg particularly had taken profound exception.

We have interest in an instance of the "perturbation problem" which is very easily stated: Assume the eigenvalues $\{E_1^0, E_2^0, ...\}$ —collectively, the "spectrum"—of \mathbf{H}^0 to be known. Subject \mathbf{H}^0 to some specified perturbation:

$$\mathbf{H}^0 \longrightarrow \mathbf{H} = \mathbf{H}^0 + \lambda \mathbf{V}$$

Describe the induced adjustment

$$\left\{E_1^0, E_2^0, \dots\right\} \longrightarrow \left\{E_1, E_2, \dots\right\}$$

of the spectrum. In the next section I sketch and criticize the method standardly brought to bear on the problem. I turn then to description of a method which is computationally much more efficient.

Computational inefficiency of the Rayleigh-Schrödinger method. Schrödinger works not from (2) but from (1). He takes both the unperturbed eigenvalues $\{E_n^0\}$ and the normalized unperturbed eigenvectors $\{|n^0)\}$ to be known

$$\mathbf{H}^{0}|n^{0}\rangle = E_{n}^{0}|n^{0}\rangle$$

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Computational inefficiency of the Rayleigh-Schrödinger method

and seeks to develop the perturbed eigenvalues/eigenvectors as power series in the dimensionless parameter λ that controls the strength of the perturbation:

$$(\mathbf{H}^{0} + \lambda \mathbf{V}) \{ |n^{0}\rangle + \lambda |n^{1}\rangle + \lambda^{2} |n^{2}\rangle + \cdots \}$$

= $\{ E_{n}^{0} + \lambda E_{n}^{1} + \lambda^{2} E_{n}^{2} + \cdots \} \{ |n^{0}\rangle + \lambda |n^{1}\rangle + \lambda^{2} |n^{2}\rangle + \cdots \}$

Termwise identification gives

$$\mathbf{H}^{0}|n^{0}\rangle = E_{n}^{0}|n^{0}\rangle \tag{3.0}$$

$$\mathbf{H}^{0}|n^{1}) + \mathbf{V}|n^{0}) = E_{n}^{0}|n^{1}) + E_{n}^{1}|n^{0})$$
(3.1)

$$\mathbf{H}^{0}|n^{2}) + \mathbf{V}|n^{1}) = E_{n}^{0}|n^{2}) + E_{n}^{1}|n^{1}) + E_{n}^{2}|n^{0})$$
(3.2)

$$\mathbf{H}^{0}|n^{3}) + \mathbf{V}|n^{2}) = E_{n}^{0}|n^{3}) + E_{n}^{1}|n^{2}) + E_{n}^{2}|n^{1}) + E_{n}^{3}|n^{0})$$
(3.3)

The program—which had been employed already by Lord Rayleigh (1842-1919)in his *Theory of Sound* (1877), and makes essential use of the *orthonormality* of the unperturbed eigenvectors—calls for solving (3) serially. Hit $(n^0|$ onto (3.1) and obtain

$$E_n^1 = (n^0 |\mathbf{V}| n^0) \tag{4.1}$$

which can be brought to all subsequent equations.

But before one can advance to (3.2) in quest of E_n^2 one must extract from (3.1) a description of $|n^1\rangle$, and it is at this point that the Rayleigh-Schrödinger scheme begins to bog down. It emerges² that one must

- distinguish cases in which E_n^0 is non-degenerate from
- cases in which E_n^0 is degenerate

and that even in the more favorable latter case the best one can achieve is

$$|n^{1}) = \sum_{m \neq n} |m^{0}) \frac{(m^{0}|\mathbf{V}|n^{0})}{E_{n}^{0} - E_{m}^{0}} + (\text{undetermined coefficient}) \cdot |n^{0})$$

so must still devise some satisfactory method for managing the "undetermined coefficient." Moreover, $|n^0\rangle + \lambda |n^1\rangle$ becomes an acceptable approximation to the perturbed eigenvector $|n\rangle$ only after it has been *normalized*, which is easy in principle, but introduces an added layer of complexity. When those hurdles have been cleared, one obtains

$$E_n^2 = \sum_{m \neq n} \frac{(n^0 |\mathbf{V}| m^0) (m^0 |\mathbf{V}| n^0)}{E_n^0 - E_m^0}$$
(4.2)

Prior to any attempt to compute the 3rd-order correction terms E_n^3 one must acquire a description of $|n^2\rangle$, and that effort leads even deeper into the bog. Various attempts have been made to bring a manageable degree of pattern to heavy calculation implicit in (3).³

² See, for example, Griffiths' Introduction to Quantum Mechanics (1995), $\S6.1.2$.

³ Several of those attempts are reviewed in my QUANTUM PERTURBATIONS (1969). Or see, for example, §11.2 in Powell & Crassmann; Chapter XVI §15 in Massiah; Chapter 17 §3 in Merzbacher's 2^{nd} edition.

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My basic criticism of the Rayleigh-Schrödinger method, in all of its variant formulations, is that to obtain a description of the p^{th} -order correction to E_n^0 it obligates one to compute $\{|n^1\rangle, |n^2\rangle, \ldots, |n^{p-1}\rangle\}$, even if one has no physical interest in the latter information. And that, for p > 2, requires great effort, even in the non-degenerate case.

Introduction to the determinantal method. Far better, I argue, to proceed directly from (2); i.e., from the statement

$$\det \| (m^0 | \mathbf{H}^0 + \lambda \mathbf{V} - E \mathbf{I} | n^0) \| = 0$$
(5)

which asks us to

• evaluate a determinant

• discover the roots of the resulting "characteristic polynomial."⁴

Both assignments become more daunting as the dimension N of the matrix (order of the characteristic polynomial) increases, but both, as I will show, can be managed so as to remain quite tractable even in the limit $N \to \infty$.

Look, by way of introduction, to the case N = 2. We agree to write

$$\|(m^{0}|\mathbf{H}^{0} - E\mathbf{I}|n^{0})\| = \mathbb{H}^{0} - E\mathbf{I} = \begin{pmatrix} E_{1}^{0} - E & 0\\ 0 & E_{2}^{0} - E \end{pmatrix}$$
$$\|(m^{0}|\lambda\mathbf{V}|n^{0})\| = \lambda \mathbb{V} = \lambda \begin{pmatrix} V_{1} & U^{*}\\ U & V_{2} \end{pmatrix}$$

 $Then^5$

$$\det(\mathbb{H}^{0} + \lambda \mathbb{V} - \underline{E}\mathbb{I}) = \underline{E}^{2} - \left[(E_{1}^{0} + \lambda V_{1}) + (E_{2}^{0} + \lambda V_{2}) \right] \underline{E} + \left[(E_{1}^{0} + \lambda V_{1}) \cdot (E_{2}^{0} + \lambda V_{2}) - \lambda^{2} U^{*} U \right] = 0$$
(6)

can be solved in closed form to give

⁴ ... which quantum physicists used to call—some still call—the "secular equation." Max Jammer's remarks in this regard (*Conceptual Development of Quantum Mechanics*, p. 215) are interesting: "Ironically, matrix mechanics, the outcome of Heisenberg's categorical rejection of orbits, had eventually to resort to the mathematics of orbital motions. The very name [given to equations like (5)] already testifies to the truth of this contention. For astronomers called an equation of this type a 'secular' equation (from the Latin *saeculum*=generation, *saeculum civile*=period of 100 years) as it enabled them to determine 'secular' (or long-period) disturbances of planetary orbits, as regards eccentricities and inclinations about their mean values."

⁵ I borrow here from my ADVANCED QUANTUM TOPICS (2000), Chapter 1: Two-state Systems, p. 39.

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which upon expansion in powers of λ gives

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

$$= E_{1}^{0} + \lambda V_{1} - \lambda^{2} \frac{U^{*}U}{E_{2}^{0} - E_{1}^{0}} + \cdots$$

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

$$= E_{2}^{0} + \lambda V_{2} + \lambda^{2} \frac{U^{*}U}{E_{2}^{0} - E_{1}^{0}} + \cdots$$

$$\left.\right\}$$

$$(8.1)$$

in the non-degenerate case $E_1^0 < E_2^0$, and

$$E_{1} = E^{0} + \frac{1}{2}\lambda \left\{ (V_{1} + V_{2}) - \sqrt{(V_{1} - V_{2})^{2} + 4U^{*}U} \right\} + \text{no terms of higher order}$$

$$E_{2} = E^{0} + \frac{1}{2}\lambda \left\{ (V_{1} + V_{2}) + \sqrt{(V_{1} - V_{2})^{2} + 4U^{*}U} \right\} + \text{no terms of higher order}$$
(8.2)

when the unperturbed spectrum is degenerate: $E_1^0 = E_2^0 \equiv E^0$. Notice that (8.1) supplies

$$E_{1}^{1} = (1|\mathbb{V}|1) \quad \text{and} \quad E_{1}^{2} = \frac{(1|\mathbb{V}|2)(2|\mathbb{V}|1)}{E_{1}^{0} - E_{2}^{0}} = \sum_{m \neq 1}^{2} \frac{(1|\mathbb{V}|m)(m|\mathbb{V}|1)}{E_{1}^{0} - E_{m}^{0}} \\ E_{2}^{1} = (2|\mathbb{V}|2) \quad \text{and} \quad E_{2}^{2} = \frac{(2|\mathbb{V}|1)(1|\mathbb{V}|2)}{E_{2}^{0} - E_{1}^{0}} = \sum_{m \neq 2}^{2} \frac{(2|\mathbb{V}|m)(m|\mathbb{V}|2)}{E_{2}^{0} - E_{m}^{0}} \end{cases}$$
(9)

and so conforms precisely to (4). Notice also that we have recovered (4.2) by direct analysis, without digressing to obtain descriptions of $\{|n^1)\}$.

These results are gratifying, but somewhat academic. For if quantum mechanical state space were 2-dimensional one would have *no need* of a time-independent perturbation theory, the characteristic equation (5) being then *exactly* soluable in all cases, by elementary means. We have shown that the exact result can be written *as though* it had emerged from perturbation theory, but that is a modest accomplishment. And to achieve it we played unfairly: we took advantage at (7) of a capability (quadratic formula) which is not available in the general case.

I show now how the argument can be reorganized so as to avoid the latter criticism. Make the substitution $E \mapsto E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$ in (6), expand in powers of λ , and set equal to zero the coefficients of ascending order. Entrusting the labor to *Mathematica*, we obtain

$$\begin{split} \lambda^0 &: \quad (E_n^0 - E_1^0)(E_n^0 - E_2^0) = 0\\ \lambda^1 &: \quad (2E_n^0 - E_1^0 - E_2^0)E_n^1 = (E_n^0 - E_1^0)V_2 + (E_n^0 - E_2^0)V_1\\ \lambda^2 &: \quad (2E_n^0 - E_1^0 - E_2^0)E_n^2 = -(E_n^1)^2 + (V_1 + V_2)E_n^1 - (V_1V_2 - U^*U) \end{split}$$

:

which we proceed to solve serially: The λ^0 -equation gives

$$E_n^0 = E_1^0$$
 else $E_n^0 = E_2^0$

The λ^1 -equation therefore supplies

$$E_1^1 = V_1 \equiv (1|\mathbb{V}|1) \quad \text{else} \quad E_2^1 = V_2 \equiv (2|\mathbb{V}|2)$$

and that information, when fed into the λ^2 -equation, gives

$$E_1^2 = \frac{U^*U}{E_1^0 - E_2^0} = \frac{(1|\mathbb{V}|2)(2|\mathbb{V}|1)}{E_1^0 - E_2^0} \quad \text{else} \quad E_2^2 = \frac{U^*U}{E_2^0 - E_1^0} = \frac{(2|\mathbb{V}|1)(1|\mathbb{V}|2)}{E_2^0 - E_1^0}$$

In the degenerate case $(E_1^0 = E_2^0 \equiv E^0)$ the λ^0 -equation gives

$$E_{n}^{0} = E^{0}$$

The λ^1 -equation now collapses into uninformative triviality (0 = 0), and the λ^2 -equation becomes

$$0 = -(E^{1})^{2} + E^{1}(V_{1} + V_{2}) - (V_{1}V_{2} - U^{*}U)$$
(10)

giving

$$E^{1} = E^{0} + \frac{1}{2}\lambda \left\{ (V_{1} + V_{2}) \pm \sqrt{(V_{1} - V_{2})^{2} + 4U^{*}U} \right\}$$

in precise agreement with (8.2). We have, in fact, managed to reproduce all of our former results without drawing upon the quadratic formula.⁶

Preparation for dimensional generalization. A long first step in that direction was taken by the argument just completed—an argument which places us in position to compute perturbed roots of characteristic equations of arbitrary order. But how are we to *obtain* the characteristic equation? How are we to evaluate $\det(\mathbb{H}^0 + \lambda \mathbb{V} - E\mathbb{I})$ when N is large, and what meaning are we to assign to that expression as $N \to \infty$?

In the unperturbed eigenbasis \mathbb{H}^0 is diagonal, so we have

$$\det(\mathbb{H}^{0} + \lambda \mathbb{V} - E\mathbb{I}) = \det(\mathbb{H}^{0} - E\mathbb{I}) \cdot \det(\mathbb{I} + \lambda \mathbb{M})$$

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

$$\det(\mathbb{H}^{0} - E\mathbb{I}) = \prod_{n=1}^{N} (E_{n} - E)$$
(11)

and attention shifts to the description of $det(\mathbb{I}+\lambda\mathbb{M})$. Look to the 2-dimensional

⁶ I do not consider its use in connection with (10) to be in violation of that statement, but rather to be an extension of the calculation which originally gave us E_1^0 and E_2^0 .

Preparation for dimensional generalization

case, where

$$\det(\mathbb{I} + \lambda \mathbb{M}) = 1 + \lambda \operatorname{tr} \mathbb{M} + \lambda^2 \det \mathbb{M}$$

Observe that

$$(\operatorname{tr} \mathbb{M})^2 = M_{11}^2 + 2M_{11}M_{22} + M_{22}^2$$

 $\operatorname{tr} \mathbb{M}^2 = M_{11}^2 + 2M_{12}M_{21} + M_{22}^2$

 \mathbf{SO}

$$\det \mathbb{M} = M_{11}M_{22} - M_{12}M_{21} = \frac{1}{2} \{ (\operatorname{tr} \mathbb{M})^2 - \operatorname{tr} \mathbb{M}^2 \} = \frac{1}{2!}\lambda^2 \begin{vmatrix} \operatorname{tr} \mathbb{M} & \operatorname{tr} \mathbb{M}^2 \\ 1 & \operatorname{tr} \mathbb{M} \end{vmatrix}$$

which we use to obtain

$$\det(\mathbb{I} + \lambda \mathbb{M}) = 1 + \lambda \operatorname{tr} \mathbb{M} + \frac{1}{2!} \lambda^2 \begin{vmatrix} \operatorname{tr} \mathbb{M} & \operatorname{tr} \mathbb{M}^2 \\ 1 & \operatorname{tr} \mathbb{M} \end{vmatrix}$$
(12)

This pretty statement is a truncated instance of a remarkable identity which deserves to be much better known, and which in higher-dimensional cases continues

$$det(\mathbb{I} + \lambda \mathbb{M}) = 1 + \lambda T_1 + \frac{1}{2!}\lambda^2 \begin{vmatrix} T_1 & T_2 \\ 1 & T_1 \end{vmatrix} + \frac{1}{3!}\lambda^3 \begin{vmatrix} T_1 & T_2 & T_3 \\ 1 & T_1 & T_2 \\ 0 & 2 & T_1 \end{vmatrix}$$
(13)
$$+ \frac{1}{4!}\lambda^4 \begin{vmatrix} T_1 & T_2 & T_3 & T_4 \\ 1 & T_1 & T_2 & T_3 \\ 0 & 2 & T_1 & T_2 \\ 0 & 0 & 3 & T_1 \end{vmatrix} + \cdots$$
$$\equiv \Delta_0 + \lambda \Delta_1 + \frac{1}{2!}\lambda^2 \Delta_2 + \frac{1}{3!}\lambda^3 \Delta_3 + \frac{1}{4!}\lambda^4 \Delta_4 + \cdots$$
(14)

with $T_p \equiv \operatorname{tr} \mathbb{M}^p$. One discovers experimentally, and can readily prove, that

$$\Delta_{0} = 1$$

$$\Delta_{1} = T_{1}$$

$$\Delta_{2} = T_{1}\Delta_{1} - T_{2}$$

$$\Delta_{3} = T_{1}\Delta_{2} - 2T_{2}\Delta_{1} + 2T_{3}$$

$$\Delta_{4} = T_{1}\Delta_{3} - 3T_{2}\Delta_{2} + 6T_{3}\Delta_{1} - 6T_{4}$$

$$\Delta_{5} = T_{1}\Delta_{4} - 4T_{2}\Delta_{3} + 12T_{3}\Delta_{2} - 24T_{4}\Delta_{1} + 24T_{5}$$

$$\Delta_{6} = T_{1}\Delta_{5} - 5T_{2}\Delta_{4} + 20T_{3}\Delta_{3} - 60T_{4}\Delta_{2} + 120T_{5}\Delta_{1} - 120T_{6}$$

$$\vdots$$

$$\Delta_{n} = \sum_{k=1}^{n} (-)^{k+1} \frac{(n-1)!}{(n-k)!} T_{k} \Delta_{n-k}$$
(15)

and by iteration we are led to the following explicit descriptions of the first few $\Delta\text{-factors:}$

$$\Delta_{0} = 1$$

$$\Delta_{1} = T_{1}$$

$$\Delta_{2} = T_{1}^{2} - T_{2}$$

$$\Delta_{3} = T_{1}^{3} - 3T_{1}T_{2} + 2T_{3}$$

$$\Delta_{4} = T_{1}^{4} - 6T_{1}^{2}T_{2} + 8T_{1}T_{3} + 3T_{2}^{2} - 6T_{4}$$

$$\Delta_{5} = T_{1}^{5} - 10T_{1}^{3}T_{2} + 20T_{1}^{2}T_{3} + 15T_{1}(T_{2}^{2} - 4T_{4}) - 20T_{2}T_{3} + 24T_{5}$$

$$\vdots$$

$$(16)$$

These results *Mathematica* has confirmed by direct evaluation of the relevant determinants. Slight recasting of (12) gives

$$\varphi(\omega) = \det(\mathbb{M} - \omega\mathbb{I}) = \omega^2 - T_1\omega + \frac{1}{2!}(T_1^2 - T_2) = \Delta_0 \omega^{2-0} - \frac{1}{1!}\Delta_1 \omega^{2-1} + \frac{1}{2!}\Delta_2 \omega^{2-2}$$

By the Cayley-Hamilton theorem $\varphi(\mathbb{M}) = \mathbb{O}$. Multiply by \mathbb{M} and take the trace, to obtain $T_3 - T_1T_2 + \frac{1}{2}(T_1^3 - T_1T_2) = \frac{1}{2}\Delta_3 = 0$. An easy extension of the argument (which makes critical use of (15)) serves to establish that

$$\Delta_{N+1} = \Delta_{N+2} = \Delta_{N+3} = \dots = 0$$
 in the N-dimensional case

and thus to explain why the 2-dimensional statement (12) presents an instance of (13) that truncates at 2^{nd} order.

For the derivation of (13) I must refer to other sources,⁷ but will sketch its principal features. Write

$$\det(\mathbb{I} + \lambda \mathbb{M}) = e^{\operatorname{tr}\left\{\log(\mathbb{I} + \lambda \mathbb{M})\right\}}$$
$$\log(\mathbb{I} + \lambda \mathbb{M}) \equiv \lambda \mathbb{M} - \frac{1}{2}(\lambda \mathbb{M})^2 + \frac{1}{3}(\lambda \mathbb{M})^3 - \frac{1}{4}(\lambda \mathbb{M})^4 + \cdots$$
$$= e^{\lambda T_1 - \frac{1}{2}\lambda^2 T_2 + \frac{1}{3}\lambda^3 T_3 - \frac{1}{4}\lambda^4 T_4 + \cdots}$$
$$\equiv e^{g(\lambda)}$$
$$= \sum \frac{1}{n!} \lambda^n \left[\left(\frac{d}{d\lambda}\right)^n e^{g(\lambda)} \right]_{\lambda=0}$$

Success hinges on one's ability to compute the n^{th} derivative of a composite function $f(g(\lambda))$. I learned to do so from Advanced Problem No. 4782 which V.F.Ivanoff submitted to the American Mathematical Monthly (**65**, 212 (1958)), but according to Abramowitz & Stegun (**24.1.2**) the basic formula is due to one Faà di Bruno (about whom I have been able to discover nothing ... but see below!), and is presumably ancient. It is, in any event, this final step that gives birth to the triangular determinants Δ_n .

⁷ See, for example, "Applications of an elegant formula due to V. F. Ivanoff" in COLLECTED SEMINARS 1963–1970; pp. 27–30 in QUANTUM PERTURBATIONS (1969); or "A mathematical note: Algorithm for the efficient evaluation of the trace of the inverse of a matrix" (1996).

Finer details

The identity (13) possesses a number of remarkable properties (for example: it simplifies markedly if \mathbb{M} is antisymmetric; also if \mathbb{M} is projective), but the feature to which I now draw special attention is that the coefficients (once "switched on" by the condition $N \ge$ order) retain their structure as N ascends. Which means (if we set aside all questions having to do with convergence) that (13) remains meaningful even in the limit $N \to \infty$!⁸

Finer details. Looking back again to (11), we are reminded that in the present application

$$\mathbb{M} = \left\| \frac{V_{ij}}{E_i - E} \right\| \quad \text{therefore} \quad \mathbb{M}^2 = \left\| \frac{V_{ij}V_{jk}}{(E_i - E)(E_j - E)} \right\|$$
$$\mathbb{M}^3 = \left\| \frac{V_{ij}V_{jk}V_{k\ell}}{(E_i - E)(E_j - E)(E_\ell - E)} \right\|, \text{ etc.}$$

which give

$$T_1(E) = \sum_{i} \frac{V_{ii}}{E_i - E}$$
(17.1)

$$T_2(E) = \sum_{ij} \frac{V_{ij}V_{ji}}{(E_i - E)(E_j - E)}$$
(17.2)

$$T_{3}(E) = \sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{(E_{i} - E)(E_{j} - E)(E_{k} - E)}$$
(17.3)

⁸ Having completed that sentence, I headed home for the evening ... ran into retired colleague Dennis Hoffman and his wife Carol on one of their daily promanades ... mentioned that I had been trying unsuccessfully since 1969 to learn something about the life of Faà di Bruno, and challenged Dennis to find trace of the man on the World Wide Web. Early the next morning Dennis appeared in my office, bearing many pages of text, from which I extract this information: Francesco Faà di Bruno (1825–1888) studied at the Royal Military Academy of Turin and served as an officer in the Sardinian Army from 1847 until, in 1953, he decided to leave the army and take up the study of mathematics. At the Sorbonne he studied under Cauchy, and was a classmate and friend of both Hermite and Leverrier (co-discoverer of Neptune). He took his doctorate from the University of Turin, and served on the faculty there from 1871 until the time of his death. In 1876 he was appointed to the Chair of Higher Analysis, but also in that same year he was ordained a Roman Catholic priest. In the latter capacity he established a religious order to attend to the needs of girls resident in an orphanage called Conservatorio del Suffragio. To keep the girls occupied he acquired a printing press and set up Tipographia Suffragio, a publishing house specializing in mathematical texts, which the girls served as typesetters. Faà di Bruno was declared a Saint by Pope John Paul II in 1988. His mathematical work treated the theory and applications of elliptic functions, the theory of errors, and (most famously) the theory of binary forms. The formula which inspires my interest in him was developed fairly early in his career, and reportedly appears in his Traite Elementaire du Calcul (1869).

Those functions, thought of as functions of a complex variable E, have poles strung along the real axis—poles situated at points specified by the unperturbed spectrum $\{E_1, E_2, \ldots\}$. Those are precisely the points at which

$$P(E) \equiv \det(\mathbb{H}^0 - E\mathbb{I}) = \prod_{i=1}^N (E_i - E)$$
$$= \left\{\prod_i E_i\right\} \cdot \left\{\prod_i \left(1 - \frac{E}{E_i}\right)\right\}$$

—the first of the factors to which (11) directed our attention—vanishes. We stand evidently in prospect of some delicate cancellations.

Consider, for a moment, the object P(E). When N is finite it is simply a polynomial with specified zeros. But in the limit $N \to \infty$ it—for most spectra $\{E_1, E_2, \ldots\}$ of physical interest—fails to converge, so might be described as "an absurdity with specified zeros." One might, for present purposes, abandon the $\prod E_i$ -factor, and try to get some mileage out of what Weierstrass had to say⁹ about the relatively convergent construction $\prod(1 - E/E_i)$, but I won't go down that road; I will instead look upon P(E) as a *formal repository of unperturbed spectral data*, and take interest in how the latent pathologies heal themselves in the intended application.

We have need of the construction

$$P(E^{0} + \lambda E^{1} + \lambda^{2} E^{2} + \cdots) = P(E^{0}) + \lambda P(E^{0}, E^{1}) + \lambda^{2} P(E^{0}, E^{1}, E^{2}) + \cdots$$
$$= P_{0} + \lambda P_{1} + \lambda^{2} P_{2} + \lambda^{3} P_{3} + \cdots$$

where

$$P_0 \equiv P(E^0) = \Pi_0(E^0) \equiv \prod (E_i - E^0)$$
(18.0)

To obtain $P_1 \equiv P(E^0, E^1)$ we write

$$(E_1-E^0-\lambda E^1-\lambda^2 E^2-\cdots)(E_2-E^0-\lambda E^1-\lambda^2 E^2-\cdots)(E_3-E^0-\lambda E^1-\lambda^2 E^2-\cdots)\cdots$$

and \bullet select an E^1 in all possible ways

• set $\lambda = 0$ in all surviving factors; this gives

$$P(E^{0}, E^{1}) = -E^{1} \sum_{i} \frac{P(E^{0})}{E_{i} - E^{0}}$$

which we abbreviate

$$P_1 = -E^1 \Pi_1 \tag{18.1}$$

 $\Pi_1(E^0) \equiv \text{sum over all ways of striking one factor from } \Pi_0$

To obtain $P_2 \equiv P(E^0, E^1, E^2)$ we first

- select E^1 then another E^1 in all possible ways, then
- select E^2 in all possible ways, always setting $\lambda = 0$ in surviving factors.

⁹ See, for example, S. Lang, *Complex Analysis* (1977), Chapter 10, §2.

Finer details

- To obtain $P_3 \equiv P(E^0, E^1, E^2, E^3)$ we first select E^1 then another E^1 then another E^1 in all possible ways, then
 - select E^1 then E^2 in all possible ways, then

• select E^3 in all possible ways.

These procedures give

To discover the terms that contribute to $P(E^0, E^1, \ldots, E^n)$ one looks to the partitions of n, which Mathematica is happy to supply: turn on the Add-On Package

<<DiscreteMath`Combinatorica`

and ask for Partitions[4] to obtain

$$\{\{1,1,1,1\},\{1,1,2\},\{1,3\},\{2,2\},\{4\}\}$$

while PartitionsP[4] responds 5 in response to the question: "In how many distinct ways can 4 be written as a sum of positive integers?" Giving names to the sums which appear recurrently in (18), and drawing upn the information just obtained, we find ourselves in position to continue the series:

$$P_1 = -E^1 \Pi_1(E^0) \tag{19.1}$$

$$P_2 = E^1 E^1 \Pi_2(E^0) - E^2 \Pi_1(E^0)$$
(19.2)

$$P_3 = -E^1 E^1 E^1 \Pi_3(E^0) + \mathbf{2} E^1 E^2 \Pi_2(E^0) - E^3 \Pi_1(E^0)$$
(19.3)

$$P_4 = E^1 E^1 E^1 E^1 \Pi_4(E^0) - 3E^1 E^1 E^2 \Pi_3(E^0)$$
(19.4)

$$+ \left\{ 2E^{1}E^{3} + E^{2}E^{2} \right\} \Pi_{2}(E^{0}) - E^{4}\Pi_{1}(E^{0})$$

In next higher order we encounter PartitionsP[5]=7 terms; they are

 $\begin{cases} 1, 1, 1, 1, 1 \\ 1, 1, 1, 2 \\ 1, 1, 3 \\ 1, 2, 2 \\ 1, 2, 2 \\ 1, 4 \\ 2, 3 \\ 5 \\ \end{cases}$

and with this information $P_5 \equiv P(E^0, E^1, E^2, E^3, E^4, E^5)$ almost writes itself. But it would be senseless to continue the process very far, since

$$p(10) = 42$$
, $p(20) = 627$, $p(30) = 5604$, $p(40) = 37338$

The series

$$P(E^{0} + \lambda E^{1} + \lambda^{2} E^{2} + \dots) = \sum_{k=0} \lambda^{k} P(E^{0}, \dots, E^{k})$$
(20)

speaks falsely when k > N, but this is no problem in the limit $N \to \infty$, and no problem even for N > about 4 if we plan to do our perturbation theory in realistic order. The boldface numerics evident in (19.3/4)—one was encountered already at (18.3)—arise from the circumstance that

- $E^1 E^2$ can be written in **2** distinct ways;
- $E^1 E^1 E^2$ can be written in **3** distinct ways;
- $E^1 E^3$ can be written in **2** distinct ways, etc.

They are, in short, multinomial coefficients. Generally

$$(E^{1} + E^{2} + \dots + E^{m})^{n} = \sum (n; n_{1}, n_{2}, \dots, n_{m}) (E^{1})^{n_{1}} (E^{2})^{n_{2}} \cdots (E^{m})^{n_{m}}$$

where the sum ranges over all partitions of n into m parts

$$n = n_1 + n_2 + \dots + n_m$$

 and^{10}

$$(n; n_1, n_2, \dots, n_m) =$$
 number of distinct arrangements
$$= \frac{(n_1 + n_2 + \dots + n_m)!}{n_1! n_2! \cdots n_m!}$$

In particular, we have $(2; 1, 1) = \frac{2!}{1!1!} = 2$ and $(3; 2, 1) = \frac{3!}{2!1!} = 3$, as reported above. I have used *Mathematica* (a fairly tedious business it was!) to check—through 4th-order in the case N = 5—the accuracy of the equation that results when (19) is introduced into (20).

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¹⁰ See Abramowitz & Stegun, **24.1.2**. *Mathematica* produces multinomial coefficients by command Multinomial $[n_1, n_2, \ldots, n_m]$.

Finer details

Return now again to (17.1), from which we obtain

$$T_1(E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots) = \sum_i \frac{V_{ii}}{E_i - E^0} \left[1 - \frac{\lambda E^1 + \lambda^2 E^2 + \cdots}{E_i - E^0} \right]^{-1}$$

Formally (meaning apart from the convergence question)

$$[\text{etc.}]^{-1} = 1 + \frac{1}{(E_i - E^0)} (\lambda E^1 + \lambda^2 E^2 + \cdots) + \frac{1}{(E_i - E^0)^2} (\lambda E^1 + \lambda^2 E^2 + \cdots)^2 + \cdots = 1 + \lambda \Big[\frac{E^1}{D_i} \Big] + \lambda^2 \Big[\frac{E^1 E^1}{D_i^2} + \frac{E^2}{D_i} \Big] + \lambda^3 \Big[\frac{E^1 E^1 E^1}{D_i^3} + \frac{2E^1 E^2}{D_i^2} + \frac{E^3}{D_i} \Big] + \lambda^4 \Big[\frac{E^1 E^1 E^1 E^1}{D_i^4} + \frac{3E^1 E^1 E^2}{D_i^3} + \frac{E^2 E^2 + 2E^1 E^3}{D_i^2} + \frac{E^4}{D_i} \Big] + \cdots$$

into which the boldface numerics have intruded for the same reason as before, and where we have adopted the abbreviation $D_i \equiv E_i - E^0$. Working similarly from $(17.2/3/\cdots)$ we find

$$T_{2}(E^{0} + \lambda E^{1} + \lambda^{2} E^{2} + \cdots) = \sum_{ij} \frac{V_{ij} V_{ji}}{D_{i} D_{j}} \left[1 - \frac{\lambda E^{1} + \lambda^{2} E^{2} + \cdots}{D_{i}} \right]^{-1} \left[1 - \frac{\lambda E^{1} + \lambda^{2} E^{2} + \cdots}{D_{j}} \right]^{-1}$$

with $[\text{etc.}]_i^{-1}[\text{etc.}]_j^{-1} = 1 + \lambda \left[\frac{E^1}{D_i} + \frac{E^1}{D_j}\right]$

$$+ \lambda^{2} \Big[\frac{E^{1}E^{1}}{D_{i}^{2}} + \frac{E^{2}}{D_{i}} + \frac{E^{1}E^{1}}{D_{j}^{2}} + \frac{E^{2}}{D_{j}} + \frac{E^{1}E^{1}}{D_{i}D_{j}} \Big] + \lambda^{3} \Big[\frac{E^{1}E^{1}E^{1}}{D_{i}^{3}} + \frac{2E^{1}E^{2}}{D_{i}^{2}} + \frac{E^{3}}{D_{i}} + \frac{E^{1}E^{1}E^{1}}{D_{j}^{3}} + \frac{2E^{1}E^{2}}{D_{j}^{2}} + \frac{E^{3}}{D_{j}} + \frac{E^{1}}{D_{j}} \Big(\frac{E^{1}E^{1}}{D_{i}^{2}} + \frac{E^{2}}{D_{i}} \Big) + \frac{E^{1}}{D_{i}} \Big(\frac{E^{1}E^{1}}{D_{j}^{2}} + \frac{E^{2}}{D_{j}} \Big) \Big] + \cdots$$

$$T_{3}(E^{0} + \lambda E^{1} + \lambda^{2} E^{2} + \cdots) = \sum_{ijk} \frac{V_{ij} V_{jk} V_{ki}}{D_{i} D_{j} D_{k}} \Big[1 - \frac{\lambda E^{1} + \lambda^{2} E^{2} + \cdots}{D_{i}} \Big]^{-1} \Big[1 - \frac{\lambda E^{1} + \lambda^{2} E^{2} + \cdots}{D_{j}} \Big]^{-1} \\ \cdot \Big[1 - \frac{\lambda E^{1} + \lambda^{2} E^{2} + \cdots}{D_{k}} \Big]^{-1}$$

$$\begin{split} \text{with} \left[\text{etc.} \right]_{i}^{-1} \left[\text{etc.} \right]_{j}^{-1} \left[\text{etc.} \right]_{k}^{-1} = 1 + \lambda \left[\frac{E^{1}}{D_{i}} + (i \mapsto j, k) \right] \\ &+ \lambda^{2} \left[\frac{E^{1}E^{1}}{D_{i}^{2}} + \frac{E^{2}}{D_{i}} + (i \mapsto j, k) \right] \\ &+ \frac{E^{1}E^{1}}{D_{i}D_{j}} + (ij \mapsto ik, jk) \right] \\ &+ \lambda^{3} \left[\frac{E^{1}E^{1}E^{1}}{D_{i}^{3}} + \frac{2E^{1}E^{2}}{D_{i}^{2}} + \frac{E^{3}}{D_{i}} + (i \mapsto j, k) \right. \\ &+ \frac{E^{1}}{D_{i}} \left(\frac{E^{1}E^{1}}{D_{j}^{2}} + \frac{E^{2}}{D_{j}} \right) + (ij \mapsto ji, ik, ki, jk, kj) \\ &+ \frac{E^{1}E^{1}E^{1}E^{1}}{D_{i}D_{j}D_{j}D_{k}} \right] + \cdots \end{split}$$

and so forth; these results¹¹ will be notated

$$T_n(E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots) = T_{n0}(E^0) + \lambda \ T_{n1}(E^0, E^1) + \lambda^2 T_{n2}(E^0, E^1, E^2) + \lambda^3 T_{n3}(E^0, E^1, E^2, E^3) + \cdots$$
(21)

to emphasize an important shared feature of their design.

Principles of assembly & information extraction. Introducing (21) into (16) we find

$$\begin{split} \Delta_0 &= 1 \\ \Delta_1 &= T_{10} + \lambda T_{11} + \lambda^2 T_{12} + \lambda^3 T_{13} + \cdots \\ \Delta_2 &= (T_{10}^2 - T_{20}) + \lambda \ (2T_{10}T_{11} - T_{21}) \\ &\quad + \lambda^2 (T_{11}^2 + 2T_{10}T_{12} - T_{22}) \\ &\quad + \lambda^3 (2T_{11}T_{12} + 2T_{10}T_{13} - T_{23}) + \cdots \\ \Delta_3 &= (T_{10}^3 - 3T_{10}T_{20} + 2T_{30}) \\ &\quad + \lambda \ (3T_{10}^2T_{11} - 3T_{11}T_{20} - T_{10}T_{21} + 2T_{31}) \\ &\quad + \lambda^2 (3T_{10}^2T_{12} - 3T_{12}T_{20} - 3T_{11}T_{21} \\ &\quad + 3T_{10}T_{11}^2 - 3T_{10}T_{22} + 2T_{32}) \cdots \\ \vdots \end{split}$$

Bringing this information to (14), we find that if

$$\mathbb{M} = \left\| \frac{V_{ij}}{E_i - (E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots)} \right\|$$
$$= \left\| \frac{V_{ij}}{E_i - E^0} \left[1 - \frac{\lambda E^1 + \lambda^2 E^2 + \cdots}{E_i - E^0} \right]^{-1} \right\|$$

 then

$$det(\mathbb{I} + \lambda \mathbb{M}) = \Delta_0 + \lambda \Delta_1 + \lambda^2 \Delta_2 + \cdots$$

= 1 + λT_{10}
+ $\frac{1}{2} \lambda^2 (T_{10}^2 + 2T_{11} - T_{20})$
+ $\frac{1}{6} \lambda^3 (T_{10}^3 + 6T_{12} + 6T_{10}T_{11} - 3T_{10}T_{20} - 3T_{21} + 2T_{30}) + \cdots$

This we use in (11)—i.e., in

$$\det \left(\mathbb{H}^0 + \lambda \mathbb{V} - (E^0 + \lambda E^1 + \lambda^2 E^2 + \cdots) \mathbb{I} \right)$$
$$= (P_0 + \lambda P_1 + \lambda^2 P_2 + \cdots) \cdot \det(\mathbb{I} + \lambda \mathbb{M}) = 0$$

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¹¹ The expressions become rapidly more complicated as one ascends to higher order, and efficient notation becomes increasingly a concern. But the work would be assigned to a computer, so we are really talking here about the design of *efficient computer algorithms*, not "efficient notation" in the classic sense.

Principles of assembly & information extraction

—to obtain

$$0 = P_0 \tag{22.0}$$

$$0 = P_1 + P_0 T_{10} \tag{22.1}$$

$$0 = P_2 + P_1 T_{10} + \frac{1}{2} P_0 (T_{10}^2 + 2T_{11} - T_{20})$$

$$0 = P_3 + P_2 T_{10} + \frac{1}{2} P_1 (T_{10}^2 + 2T_{11} - T_{20})$$
(22.2)

$$+ \frac{1}{6}P_0(T_{10}^3 + 6T_{12} + 6T_{10}T_{11} - 3T_{10}T_{20} - 3T_{21} + 2T_{30})$$
(22.3)

which we undertake to solve serially.

The 0th condition, when spelled out with the aid of (18.0), forces E^0 to be one or another of the unperturbed eigenvalues; we will set

$$E^0 = E_n \tag{23.0}$$

That brings about great simplifications that ripple downstream. First off, (23.0) serves to kill all but one of the terms which enter summed into the definition (18.1) of Π_1 ; we therefore have

$$P_1 = -E_n^1 \prod_{k \neq n} D_{kn} \quad \text{with} \quad D_{kn} \equiv E_k - E_n$$

Equation (22.1) therefore becomes

which in the finite-dimensional case we can—and even in the ∞ -dimensional will—interpret to mean that

$$E_n^1 = V_{nn} \tag{23.1}$$

provided the unperturbed eigenvalue E_n is non-degenerate; in the contrary case we have 0 = 0 and (as we saw already in the case N = 2) must look farther downstream for the information required to evaluate E_n^1 .

But as we move downstream the principles of inclusion/exclusion implicit in expressions of rapidly ascending complexity become increasingly difficult to sort out. I have found it convenient to have at hand an explicit instance of what those principles are trying to tell us. So take N = 5, and let the unperturbed eigenvalues be denoted $\{E_1, E_2, E_3, E_4, E_n\}$. Then¹²

$$\Pi_{0}(E_{n}) = D_{1n}D_{2n}D_{3n}D_{4n}D_{nn}$$

$$\Pi_{1}(E_{n}) = D_{1n}D_{2n}D_{3n}D_{4n} + D_{1n}D_{2n}D_{3n}D_{nn}$$

$$+ D_{1n}D_{2n}D_{4n}D_{nn}$$

$$+ D_{1n}D_{3n}D_{4n}D_{nn}$$

$$+ D_{2n}D_{3n}D_{4n}D_{nn}$$

$$\Pi_{2}(E_{n}) = D_{1n}D_{2n}D_{3n} + D_{1n}D_{2n}D_{4n} + D_{1n}D_{3n}D_{4n} + D_{2n}D_{3n}D_{4n} + D_{1n}D_{2n}D_{nn} + D_{1n}D_{3n}D_{nn} + D_{1n}D_{4n}D_{nn} + D_{2n}D_{3n}D_{nn} + D_{2n}D_{4n}D_{nn} + D_{3n}D_{4n}D_{nn}$$

 $\Pi_{3}(E_{n}) = D_{1n}D_{2n} + D_{1n}D_{3n} + D_{1n}D_{4n} + D_{2n}D_{3n} + D_{2n}D_{4n} + D_{3n}D_{4n} + D_{1n}D_{nn} + D_{2n}D_{nn} + D_{3n}D_{nn} + D_{4n}D_{nn}$

$$\Pi_4(E_n) = D_{1n} + D_{2n} + D_{3n} + D_{4n} + D_{nn}$$

The terms with red factors vanish when they stand alone or are divided by D_{kn} , but make non-vanishing contributions when divided by D_{nn} . We have already seen this happen : (22.1), in the present expanded notation, reads

$$0 = -E_n^1 \left\{ (\text{quartic term}) + (\text{cubic terms}) D_{nn} \right\}$$
$$+ (\text{quartic term}) D_{nn} \left\{ \sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}} \right\}$$
$$= \underbrace{\left\{ -E_n^1 + V_{nn} \right\}}_{i} \cdot (\text{quartic term})$$

0 unless spectral value E_n is degenerate: (quartic term) = 0

We look now in that same spirit to the implications of (22.2), which asks us to add terms of five distinct types. I look to those terms separately:

FIRST TERM: SECOND ORDER

$$P_{2} = (E_{n}^{1})^{2}\Pi_{2}(E_{n}) - E_{n}^{2}\Pi_{1}(E_{n}) \text{ by (19.2)}$$

$$= (E_{n}^{1})^{2} \Big\{ (\text{cubic terms}) + (\text{quadratic terms})D_{nn} \Big\}$$

$$- E_{n}^{2} \Big\{ (\text{quartic term}) + (\text{cubic terms})D_{nn} \Big\}$$

$$\downarrow$$

$$= (E_{n}^{1})^{2} (\text{cubic terms}) - E_{n}^{2} (\text{quartic term})$$

¹² The reader should be aware that in the electronic version of this text all D_{nn} 's are red, and that I use blue to distinguish factors that come into being as coefficients of D_{nn} from those that don't.

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SECOND TERM: SECOND ORDER $P_1 T_{10} = -E_n^1 \Pi_1(E_n) T_{01}(E_n)$ $= -E_n^1 \bigg\{ (\text{quartic term}) + (\text{cubic terms}) D_{nn} \bigg\} \bigg\{ \sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}} \bigg\}$ $\stackrel{\Psi}{=} -\left\{ E_n^1(\text{quartic term}) \sum_i \frac{V_{ii}}{D_{in}} + E_n^1 V_{nn}(\text{cubic terms}) \right\} - E_n^1 V_{nn} \frac{(\text{quartic term})}{D_{nn}}$ THIRD TERM: SECOND ORDER $\frac{1}{2}P_0T_{10}^2 = \frac{1}{2}\Pi_0(E_n)[T_{10}(E_n)]^2$ $= \frac{1}{2} (\text{quartic term}) \frac{D_{nn}}{D_{in}} \left[\sum_{i} \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}} \right]^2$ $= (\text{stuff}) \frac{D_{nn}}{D_{nn}} + V_{nn} \sum_{i} V_{ii} \frac{(\text{quartic term})}{D_{in}} + \frac{1}{2} V_{nn} V_{nn} \frac{(\text{quartic term})}{D_{nn}}$ $= V_{nn} (\text{quartic term}) \sum_{i} \frac{V_{ii}}{D_{in}} + \frac{1}{2} V_{nn} V_{nn} \frac{(\text{quartic term})}{D_{nn}}$ FOURTH TERM: SECOND ORDER $P_0 T_{11} = \Pi_0(E_n) T_{11}(E_n, E_n^1)$ $= (\text{quartic term}) D_{nn} \left\{ E_n^1 \sum_i \frac{V_{ii}}{D_{in} D_{in}} + \frac{E_n^1 V_{nn}}{D_{nn} D_{nn}} \right\}$ $= (\text{stuff}) \underline{D_{nn}} + E_n^1 V_{nn} \frac{(\text{quartic term})}{\underline{D_{nn}}}$ $\stackrel{\Psi}{=} E_n^1 V_{nn} \frac{(\text{quartic term})}{D_{nn}}$ FIFTH TERM: SECOND ORDER

$$\begin{aligned} -\frac{1}{2}P_0T_{20} &= -\frac{1}{2}\Pi_0(E_n)T_{20}(E_n) \\ &= -\frac{1}{2}(\text{quartic term})D_{nn} \\ &\cdot \left\{\sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_i \frac{V_{ni}V_{in}}{D_{in}D_{nn}} + \frac{V_{nn}V_{nn}}{D_{nn}D_{nn}}\right\} \\ &= (\text{stuff})D_{nn} - (\text{quartic term})\sum_i \frac{V_{ni}V_{in}}{D_{in}} - \frac{1}{2}V_{nn}V_{nn}\frac{(\text{quartic term})}{D_{nn}} \\ &\downarrow \\ &= -(\text{quartic term})\sum_i \frac{V_{ni}V_{in}}{D_{in}} - \frac{1}{2}V_{nn}V_{nn}\frac{(\text{quartic term})}{D_{nn}} \end{aligned}$$

Summing up those five terms, we are led from (22.2) to an equation of the form

$$0 = \sum \text{FIVE TERMS}$$
$$= \text{GOOD STUFF}_{2} + \text{STUFF}_{2,1} \frac{1}{D_{nr}}$$

Preserving the sequential order of the terms that contribute to the coefficient of $(D_{nn})^{-1}$ we find

$$\underbrace{\text{STUFF}}_{2,1} = (0 - 1 + 0 + 1 + 0) \cdot (\text{quartic term}) E_n^1 V_{nn} \\ + (0 + 0 + \frac{1}{2} + 0 - \frac{1}{2}) \cdot (\text{quartic term}) V_{nn} V_{nn} = 0$$

This result protects us from a catastrophy of class ∞^1 , and inspires some confidence in the accuracy of our work. Look next to GOOD STUFF₂, which we find can be expressed¹³

$$\overline{\text{GOOD STUFF}}_{2} = (\text{quartic}) \left\{ -E_{n}^{2} - \sum_{i} \frac{V_{ni}V_{in}}{D_{in}} - \left[E_{n}^{1} - V_{nn}\right] \sum_{i} \frac{V_{ii}}{D_{in}} \right\}$$
$$+ (\text{cubic}) E_{n}^{1} \left[E_{n}^{1} - V_{nn}\right]$$

In the non-degenerate case $[E_n^1 - V_{nn}] = 0$, and we led to the familiar 2nd-order spectral correction formula¹⁴

$$E_n^2 = -\sum_{i \neq n} \frac{V_{ni} V_{in}}{E_i^0 - E_n^0}$$
(23.2)

I remarked earlier (see the text preceding (18)) that we would "take interest in how the latent pathologies heal themselves." The mechanism stands now revealed: the potential embarrassment of an infinite $1/D_{nn}$ term was avoided when a vanishing coefficient killed the term in question. The lesson—for which

¹³ It becomes important at this point to recognize that, while I found it convenient to draw certain color-coded distinctions in the equations that (on p.16) served to described Π_0 , Π_1 , etc., they are in all cases <u>distinctions without</u> <u>a difference</u>: (cubic) and (cubic) refer to identitical expressions (namely, the sum of all distinct third-order products of non-repeating factors that include no D_{nn}), and the same can be said of (quadratic/quadratic), etc. Here and henceforth I will abandon the blue ink when it obscures (instead of clarifies) what's going on.

¹⁴ See Griffiths, p. 226; Powell & Crassmann, p. 387. Notice that hermiticity forces all numerators to be positive, and that if E_n refers to thet ground state then so also are all denominators positive. One is brought thus to the familiar conclusion that <u>perturbation always serves in second order to *lower* the ground state.</u>

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a good rationale could be given—appears to be this: first complete all the algebra, and only then turn on the condition $D_{nn} \mapsto 0$.

Look finally to the implications of (22.3), which—no small request!—asks us to develop and sum terms of the following eleven species:

FIRST TERM: THIRD ORDER

$$\begin{split} P_{3} &= -(E_{n}^{1})^{3}\Pi_{3} + 2E_{n}^{1}E_{n}^{2}\Pi_{2} - E_{n}^{3}\Pi_{1} \\ &= -(E_{n}^{1})^{3}\Big\{(\text{quadratic terms}) + (\text{linear terms})D_{nn}\Big\} \\ &+ 2E_{n}^{1}E_{n}^{2}\Big\{(\text{cubic terms}) + (\text{quadratic terms})D_{nn}\Big\} \\ &- E_{n}^{3}\Big\{(\text{quartic term}) + (\text{cubic terms})D_{nn}\Big\} \\ &\Downarrow \\ &= -(E_{n}^{1})^{3}(\text{quadratic terms}) + 2E_{n}^{1}E_{n}^{2}(\text{cubic terms}) - E_{n}^{3}(\text{quartic term}) \end{split}$$

SECOND TERM: THIRD ORDER

$$P_{2}T_{10} = \left\{ (E_{n}^{1})^{2}\Pi_{2} - E_{n}^{2}\Pi_{1} \right\} T_{10}$$

$$= \left\{ (E_{n}^{1})^{2} \left\{ (\text{cubic terms}) + (\text{quadratic terms})D_{nn} \right\} \right\}$$

$$- E_{n}^{2} \left\{ (\text{quartic term}) + (\text{cubic terms})D_{nn} \right\} \right\} \left\{ \sum_{i} \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}} \right\}$$

$$\downarrow$$

$$= \left\{ (E_{n}^{1})^{2} (\text{cubic terms}) - E_{n}^{2} (\text{quartic term}) \right\} \sum_{i} \frac{V_{ii}}{D_{in}}$$

$$+ \left\{ (E_{n}^{1})^{2} (\text{quadratic terms}) - E_{n}^{2} (\text{quartic terms}) \right\} V_{nn}$$

$$+ \left\{ (E_{n}^{1})^{2} (\text{cubic terms}) - E_{n}^{2} (\text{quartic terms}) \right\} V_{nn} \frac{1}{D_{nn}}$$

THIRD TERM: THIRD ORDER

$$\begin{split} \frac{1}{2}P_1T_{10}^2 &= -\frac{1}{2}E_n^1\Pi_1T_{10}^2 \\ &= -\frac{1}{2}E_n^1\Big\{(\text{quartic term}) + (\text{cubic terms})D_{nn}\Big\}\Big[\sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}}\Big]^2 \\ &\downarrow \\ &= -\frac{1}{2}E_n^1\Big\{(\text{quartic term})\sum_{ij}\frac{V_{ii}V_{jj}}{D_{in}D_{jn}} + (\text{cubic terms})2V_{nn}\sum_i\frac{V_{ii}}{D_{in}}\Big\} \\ &- \frac{1}{2}E_n^1\Big\{(\text{quartic term})2V_{nn}\sum_i\frac{V_{ii}}{D_{in}} + (\text{cubic terms})V_{nn}V_{nn}\Big\}\frac{1}{D_{nn}} \\ &- \frac{1}{2}E_n^1\Big\{(\text{quartic term})V_{nn}V_{nn}\Big\}\frac{1}{D_{nn}D_{nn}} \end{split}$$

FOURTH TERM: THIRD ORDER

$$P_{1}T_{11} = -E_{n}^{1}\Pi_{1}T_{11}$$

$$= -E_{n}^{1}\left\{(\text{quartic term}) + (\text{cubic terms})D_{nn}\right\}$$

$$\cdot E_{n}^{1}\left\{\sum_{i}\frac{V_{ii}}{D_{in}D_{in}} + \frac{V_{nn}}{D_{nn}D_{nn}}\right\}$$

$$\Downarrow$$

$$= -(E_{n}^{1})^{2}\left\{(\text{quartic term})\sum_{i}\frac{V_{ii}}{D_{in}D_{in}}\right\}$$

$$- (E_{n}^{1})^{2}\left\{(\text{cubic terms})V_{nn}\right\}\frac{1}{D_{nn}}$$

$$- (E_{n}^{1})^{2}\left\{(\text{quartic term})V_{nn}\right\}\frac{1}{D_{nn}}$$

FIFTH TERM: THIRD ORDER

$$\begin{aligned} -\frac{1}{2}P_{1}T_{20} &= \frac{1}{2}E_{n}^{1}\Pi_{1}T_{20} \\ &= \frac{1}{2}E_{n}^{1}\Big\{(\text{quartic term}) + (\text{cubic terms})D_{nn}\Big\} \\ &\quad \cdot \Big\{\sum_{ij}\frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_{i}\frac{V_{ni}V_{in}}{D_{in}D_{nn}} + \frac{V_{nn}V_{nn}}{D_{nn}D_{nn}}\Big\} \\ &\downarrow \\ &= \frac{1}{2}E_{n}^{1}\Big\{(\text{quartic term})\sum_{ij}\frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + (\text{cubic terms})2\sum_{i}\frac{V_{ni}V_{in}}{D_{in}}\Big\} \\ &\quad + \frac{1}{2}E_{n}^{1}\Big\{(\text{quartic term})2\sum_{i}\frac{V_{ni}V_{in}}{D_{in}} + (\text{cubic terms})V_{nn}V_{nn}\Big\}\frac{1}{D_{nn}} \\ &\quad + \frac{1}{2}E_{n}^{1}\Big\{(\text{quartic term})V_{nn}V_{nn}\Big\}\frac{1}{D_{nn}D_{nn}} \end{aligned}$$

SIXTH TERM: THIRD ORDER

$$\begin{split} \frac{1}{6}P_0T_{10}^3 &= \frac{1}{6}\Pi_0T_{10}^3 \\ &= \frac{1}{6}(\text{quartic term})D_{nn}\left[\sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}}\right]^3 \\ &\downarrow \\ &= \frac{1}{2}\left\{(\text{quartic term})V_{nn}\sum_{ij}\frac{V_{ii}V_{jj}}{D_{in}D_{jn}}\right\} \\ &+ \frac{1}{2}\left\{(\text{quartic term})V_{nn}V_{nn}\sum_i \frac{V_{ii}}{D_{in}}\right\}\frac{1}{D_{nn}} \\ &+ \frac{1}{6}\left\{(\text{quartic term})V_{nn}V_{nn}V_{nn}\right\}\frac{1}{D_{nn}D_{nn}} \end{split}$$

SEVENTH TERM: THIRD ORDER

$$\begin{split} P_0 T_{12} &= \Pi_0 T_{12} \\ &= (\text{quartic term}) D_{nn} \\ &\quad \cdot \left\{ (E_n^1)^2 \left[\sum_i \frac{V_{ii}}{D_{in} D_{in} D_{in}} + \frac{V_{nn}}{D_{nn} D_{nn} D_{nn}} \right] \\ &\quad + E_n^2 \left[\sum_i \frac{V_{ii}}{D_{in} D_{in}} + \frac{V_{nn}}{D_{nn} D_{nn}} \right] \right\} \\ &\downarrow \\ &\downarrow \\ &= \left\{ (\text{quartic term}) E_n^2 V_{nn} \right\} \frac{1}{D_{nn}} \\ &\quad + \left\{ (\text{quartic term}) (E_n^1)^2 V_{nn} \right\} \frac{1}{D_{nn} D_{nn}} \end{split}$$

EIGHTH TERM: THIRD ORDER

$$P_0 T_{10} T_{11} = \Pi_0 T_{10} T_{11}$$

$$= (\text{quartic term}) D_{nn} \left\{ \sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}} \right\}$$

$$\cdot E_n^1 \left\{ \sum_i \frac{V_{ii}}{D_{in} D_{in}} + \frac{V_{nn}}{D_{nn} D_{nn}} \right\}$$

$$\Downarrow$$

$$= \left\{ (\text{quartic term}) E_n^1 V_{nn} \sum_i \frac{V_{ii}}{D_{in} D_{in}} \right\}$$

$$+ \left\{ (\text{quartic term}) E_n^1 V_{nn} \sum_i \frac{V_{ii}}{D_{in}} \right\} \frac{1}{D_{nn}}$$

$$+ \left\{ (\text{quartic term}) E_n^1 V_{nn} V_{nn} \right\} \frac{1}{D_{nn} D_{nn}}$$

NINTH TERM: THIRD ORDER

$$\begin{aligned} -\frac{1}{2}P_0T_{10}T_{20} &= -\frac{1}{2}\Pi_0T_{10}T_{20} \\ &= -\frac{1}{2}(\text{quartic term})D_{nn}\left\{\sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{nn}}{D_{nn}}\right\} \\ &\quad \cdot \left\{\sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_i \frac{V_{ni}V_{in}}{D_{in}D_{nn}} + \frac{V_{nn}V_{nn}}{D_{nn}D_{nn}}\right\} \\ &\downarrow \\ &= -\frac{1}{2}(\text{quartic term})\left\{V_{nn}\sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} + 2\sum_i \frac{V_{ii}}{D_{in}} \cdot \sum_j \frac{V_{nj}V_{jn}}{D_{jn}}\right\} \\ &\quad -\frac{1}{2}(\text{quartic term})\left\{2V_{nn}\sum_i \frac{V_{ni}V_{in}}{D_{in}} + V_{nn}V_{nn}\sum_i \frac{V_{ii}}{D_{in}}\right\} \frac{1}{D_{nn}} \\ &\quad -\frac{1}{2}(\text{quartic term})\left\{V_{nn}V_{nn}V_{nn}\right\} \frac{1}{D_{nn}D_{nn}} \end{aligned}$$

$$\begin{aligned} -\frac{1}{2}P_0T_{21} &= -\frac{1}{2}\Pi_0T_{21} \\ &= -\frac{1}{2}(\text{quartic term})D_{nn} \\ &\cdot \left\{\sum_{ij} \frac{V_{ij}V_{ji}}{D_{in}D_{jn}} \left[\frac{E_n^1}{D_{in}} + \frac{E_n^1}{D_{jn}}\right] + 2\sum_i \frac{V_{ni}V_{in}}{D_{in}D_{nn}} \left[\frac{E_n^1}{D_{in}} + \frac{E_n^1}{D_{nn}}\right] \\ &+ 2E_n^1V_{nn}V_{nn}\frac{1}{D_{nn}D_{nn}D_{nn}}\right\} \\ &\Downarrow \\ &= -\frac{1}{2}(\text{quartic term})\left\{2E^1\sum_i \frac{V_{ni}V_{in}}{V_{in}}\right\} \end{aligned}$$

$$= -\frac{1}{2} (\text{quartic term}) \left\{ 2E_n^1 \sum_i \frac{m}{D_{in}D_{in}} \right\}$$
$$-\frac{1}{2} (\text{quartic term}) \left\{ 2E_n^1 \sum_i \frac{V_{ni}V_{in}}{D_{in}} \right\} \frac{1}{D_{nn}}$$
$$-\frac{1}{2} (\text{quartic term}) \left\{ 2E_n^1 V_{nn} V_{nn} \right\} \frac{1}{D_{nn}D_{nn}}$$

ELEVENTH TERM: THIRD ORDER

$$\begin{split} \frac{1}{3}P_0T_{30} &= \frac{1}{3}\Pi_0T_{30} \\ &= \frac{1}{3}(\text{quartic term})D_{nn} \\ &\cdot \left\{\sum_{ijk} \frac{V_{ij}V_{jk}V_{ki}}{D_{in}D_{jn}D_{kn}} + 3\sum_{ij} \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}D_{nn}} \right. \\ &+ 3V_{nn}\sum_{i} \frac{V_{ni}V_{in}}{D_{in}D_{nn}D_{nn}} + \frac{V_{nn}V_{nn}V_{nn}}{D_{nn}D_{nn}D_{nn}}\right\} \\ &\downarrow \\ &= (\text{quartic term})\left\{\sum_{ij} \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}}\right\} \\ &+ (\text{quartic term})\left\{V_{nn}\sum_{i} \frac{V_{ni}V_{in}}{D_{in}}\right\}\frac{1}{D_{nn}} \\ &+ \frac{1}{3}(\text{quartic term})\left\{V_{nn}V_{nn}V_{nn}\right\}\frac{1}{D_{nn}D_{nn}} \end{split}$$

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Summing up those eleven terms, we are led from (22.3) to an equation of the form

$$0 = \sum \text{Eleven terms}$$

= GOOD STUFF 3 + STUFF 3,1 $\frac{1}{D_{nn}}$ + STUFF 3,2 $\frac{1}{D_{nn}D_{nn}}$

Preserving the sequential order of the terms that contribute to the coefficient of $(D_{nn})^{-2}$ we find

$$\boxed{\textbf{STUFF}}_{3,2} = 0 + 0 - \frac{1}{2}E_n^1 \left\{ (\text{quartic term})V_{nn}V_{nn} \right\} \\ - (E_n^1)^2 \left\{ (\text{quartic term})V_{nn} \right\} \\ + \frac{1}{2}E_n^1 \left\{ (\text{quartic term})V_{nn}V_{nn} \right\} \\ + \frac{1}{6} \left\{ (\text{quartic term})V_{nn}V_{nn}V_{nn} \right\} \\ + \frac{1}{6} \left\{ (\text{quartic term})(E_n^1)^2 V_{nn} \right\} \\ + \left\{ (\text{quartic term})(E_n^1)^2 V_{nn} \right\} \\ + \left\{ (\text{quartic term})E_n^1 V_{nn}V_{nn} \right\} \\ - \frac{1}{2}(\text{quartic term}) \left\{ V_{nn}V_{nn}V_{nn} \right\} \\ - \frac{1}{2}(\text{quartic term}) \left\{ 2E_n^1 V_{nn}V_{nn} \right\} \\ + \frac{1}{3}(\text{quartic term}) \left\{ V_{nn}V_{nn}V_{nn} \right\}$$

The sum on the right presents terms of three types (which would collapse into a single type if we were to draw upon $E_n^1 = V_{nn}$). Grouping terms according to type, and presenting them in such a way as to preserve sequential order, we find that <u>STUFF</u>_{3,2} can be described

$$(0+0+0+0+0+\frac{1}{6}+0+0-\frac{1}{2}+0+\frac{1}{3}) \cdot (\text{quartic})V_{nn}V_{nn}V_{nn} + (0+0-\frac{1}{2}+0+\frac{1}{2}+0+0+1+0-1+0) \cdot (\text{quartic})E_n^1V_{nn}V_{nn} + (0+0+0-1+0+0+1+0+0+0+0) \cdot (\text{quartic})(E_n^1)^2V_{nn}$$

In short:

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

This result protects us from a catastrophy of class ∞^2 , and inspires increased confidence in the accuracy of our work.

Look now to the terms that enter as coefficients of $(D_{nn})^{-1}$:

$$\begin{split} \boxed{\text{STUFF}}_{3,1} &= 0 + \left\{ (E_n^1)^2 (\text{cubic terms}) - E_n^2 (\text{quartic term}) \right\} V_{nn} \\ &\quad - \frac{1}{2} E_n^1 \left\{ (\text{quartic term}) 2V_{nn} \sum_i \frac{V_{ii}}{D_{in}} + (\text{cubic terms}) V_{nn} V_{nn} \right\} \\ &\quad - (E_n^1)^2 \left\{ (\text{cubic terms}) V_{nn} \right\} \\ &\quad + \frac{1}{2} E_n^1 \left\{ (\text{quartic term}) 2 \sum_i \frac{V_{ni} V_{in}}{D_{in}} + (\text{cubic terms}) V_{nn} V_{nn} \right\} \\ &\quad + \frac{1}{2} \left\{ (\text{quartic term}) V_{nn} V_{nn} \sum_i \frac{V_{ii}}{D_{in}} \right\} \\ &\quad + \left\{ (\text{quartic term}) E_n^2 V_{nn} \right\} \\ &\quad + \left\{ (\text{quartic term}) E_n^1 V_{nn} \sum_i \frac{V_{ii}}{D_{in}} \right\} \\ &\quad - \frac{1}{2} (\text{quartic term}) \left\{ 2V_{nn} \sum_i \frac{V_{ni} V_{in}}{D_{in}} + V_{nn} V_{nn} \sum_i \frac{V_{ii}}{D_{in}} \right\} \\ &\quad - \frac{1}{2} (\text{quartic term}) \left\{ 2E_n^1 \sum_i \frac{V_{ni} V_{in}}{D_{in}} \right\} \\ &\quad + (\text{quartic term}) \left\{ V_{nn} \sum_i \frac{V_{ni} V_{in}}{D_{in}} \right\} \end{split}$$

The sum on the right presents terms now of seven types (which would collapse into three if we were to draw upon what we now know about E_n^1 and E_n^2). Again grouping terms according to type, and adhering to our former practice of displaying terms in a manner which respects sequential order (and thus permits us to tell where each term came from, how each cancellation comes about), we find that <u>STUFF</u>_{3,1} can be described

$$\begin{split} & \left(0-1+0+0+0+0+1+0+0+0+0\right)(\text{quartic})V_{nn}E_m^2 \\ & + \left(0+0+0+0+0+0+0+0+0-1+0+1\right)(\text{quartic})V_{nn}\sum_i V_{ni}V_{in}/D_{in} \\ & + \left(0+0+0+0+1+0+0+0+0-1+0\right)(\text{quartic})E_n^1\sum_i V_{ni}V_{in}/D_{in} \\ & + \left(0+1+0-1+0+0+0+0+0+0+0+0\right)(\text{cubic})V_{nn}(E_n^1)^2 \\ & + \left(0+0-\frac{1}{2}+0+\frac{1}{2}+0+0+0+0+0+0+0\right)(\text{cubic})V_{nn}E_n^1 \\ & + \left(0+0+0+0+0+\frac{1}{2}+0+0+0-\frac{1}{2}+0\right)(\text{quartic})V_{nn}V_{nn}\sum_i V_{ii}/D_{in} \\ & + \left(0+0-1+0+0+0+0+1+0+0+0\right)(\text{quartic})V_{nn}E_n^1\sum_i V_{ii}/D_{in} \end{split}$$

In short:

STUFF
$$_{3,1} = 0$$

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which protects us from a catastrophy of class ∞^1 . Notice that here once again we were able to obtain detailed cancellation *without* drawing upon what we (in the non-degenerate case) know about E_n^1 and E_n^2 .

I interpret $[\text{STUFF}]_{2,1} = [\text{STUFF}]_{3,1} = [\text{STUFF}]_{3,2} = 0$ to indicate that were we to work out the detailed meaning of (22.n) we would in every case obtain an equation of the design

$$P_{N} + \dots = \boxed{\text{GOOD STUFF}}_{N} + \sum_{k=1}^{N-1} \boxed{\text{STUFF}}_{N,k} (D_{nn})^{-k} = 0$$

and would in very case discover that, as a result of massive cancellation,

$$\boxed{\text{STUFF}}_{N,k} = 0$$

But I will not attempt to construct an explicit proof of a proposition the truth of which is, after all, evident on other grounds.¹⁵

It is (in the non-degenerate case) from

GOOD STUFF
$$_{N} \equiv Q_{N}(E_{n}, E_{n}^{1}, \dots, E_{n}^{N}) = 0$$

that one undertakes to extract E_n^N . We have already established that

$$Q_1(E_n^1) = \left\{ -E_n^1 + V_{nn} \right\} \cdot \prod_{k \neq n} (E_k - E_n)$$
$$Q_2(E_n^1, E_n^2) = \left\{ -E_n^2 - \sum_i \frac{V_{ni}V_{in}}{D_{in}} \right\} \cdot \prod_{k \neq n} (E_k - E_n)$$

What do the results now in hand have to say about $Q_3(E_n^1, E_n^2, E_n^3)$? Collecting the terms proportional to $(D_{nn})^0$ we find that GOOD STUFF $_3 = 0$ can be expressed

 $^{^{15}}$ The intricacy of the pattern of cancellations suggests that direct proof would be quite difficult.

$$\begin{split} 0 &= - (E_n^1)^3 (\text{quadratic}) + 2E_n^1 E_n^2(\text{cubic}) - E_n^3(\text{quartic}) \\ &+ \left\{ (E_n^1)^2(\text{cubic}) - E_n^2(\text{quartic}) \right\} \sum_i \frac{V_{ii}}{D_{in}} \\ &+ \left\{ (E_n^1)^2(\text{quadratic}) - E_n^2(\text{cubic}) \right\} V_{nn} \\ &- \frac{1}{2} E_n^1 \left\{ (\text{quartic}) \sum_{ij} \frac{V_{ii} V_{jj}}{D_{in} D_{jn}} + (\text{cubic}) 2V_{nn} \sum_i \frac{V_{ii}}{D_{in}} \right\} \\ &- (E_n^1)^2 \left\{ (\text{quartic}) \sum_i \frac{V_{ij}}{D_{in} D_{jn}} \right\} \\ &+ \frac{1}{2} E_n^1 \left\{ (\text{quartic}) \sum_{ij} \frac{V_{ii} V_{ji}}{D_{in} D_{jn}} + (\text{cubic}) 2 \sum_i \frac{V_{ni} V_{in}}{D_{in}} \right\} \\ &+ \frac{1}{2} \left\{ (\text{quartic}) V_{nn} \sum_{ij} \frac{V_{ii} V_{jj}}{D_{in} D_{jn}} \right\} \\ &+ \frac{1}{2} \left\{ (\text{quartic}) V_{nn} \sum_i \frac{V_{ii} V_{jj}}{D_{in} D_{jn}} \right\} \\ &+ 0 \\ &+ \left\{ (\text{quartic}) E_n^1 V_{nn} \sum_i \frac{V_{ii}}{D_{in} D_{jn}} \right\} \\ &- \frac{1}{2} (\text{quartic}) \left\{ V_{nn} \sum_{ij} \frac{V_{ij} V_{ji}}{D_{in} D_{jn}} + 2 \sum_i \frac{V_{ii}}{D_{in}} \cdot \sum_j \frac{V_{nj} V_{jn}}{D_{jn}} \right\} \\ &- \frac{1}{2} (\text{quartic}) \left\{ 2E_n^1 \sum_i \frac{V_{ni} V_{in}}{D_{in} D_{jn}} \right\} \\ &+ (\text{quartic}) \left\{ \sum_{ij} \frac{V_{ni} V_{ij}}{D_{in} D_{jn}} \right\} \end{split}$$

Collecting together the quadratic terms, we have

$$(\text{quadratic}) \cdot (E_n^1)^2 \left[-E_n^1 + V_{nn} \right]$$

which vanishes in consequence of what is already known about E_n^1 . Similarly we have

$$(\text{cubic}) \cdot \left\{ E_n^2 \Big[E_n^1 - V_{nn} \Big] + E_n^1 \Big[E_n^2 + \sum_i \frac{V_{ni} V_{in}}{D_{in}} \Big] + E_n^1 \Big[E_n^1 - V_{nn} \Big] \sum_i \frac{V_{ii}}{D_{in}} \right\}$$

which vanishes in consequence of what is already known about E_n^1 and E_n^2 . The surviving terms are all proportional to (quartic): after some reorganization we

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are led to a result which can be written

$$\boxed{\text{GOOD STUFF}}_{3} = \left\{ -E_n^3 + \sum_{ij} \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}} - E_n^1 \sum_i \frac{V_{ni}V_{in}}{D_{in}D_{in}} - \left[E_n^2 + \sum_i \frac{V_{ni}V_{in}}{D_{in}} \right] \sum_k \frac{V_{kk}}{D_{kn}} - E_n^1 \left[E_n^1 - V_{nn} \right] \sum_k \frac{V_{kk}}{D_{kn}D_{kn}} + \frac{1}{2} \left[E_n^1 - V_{nn} \right] \sum_{ij} \frac{V_{ij}V_{ji} - V_{ii}V_{jj}}{D_{in}D_{jn}} \right\} \cdot \prod_{k \neq n} (E_k - E_n)$$
$$\equiv Q_3(E_n^1, E_n^2, E_n^3)$$

If E_n is non-degenerate (i.e., if $\prod_{k \neq n} (E_k - E_n) \neq 0$) then the factors [etc.] vanish, and from $Q_3 = 0$ we obtain

$$E_n^3 = \sum_{i,j \neq n} \frac{V_{ni} V_{ij} V_{jn}}{D_{in} D_{jn}} - E_n^1 \cdot \sum_{i \neq n} \frac{V_{ni} V_{in}}{D_{in} D_{in}}$$
(23.3)

To recapitulate: we have (with labor) found that when spelled out in detail the meanings of (22) can, in the non-degenerate case, be expressed

$$0 = (\text{quartic}) \left[E_n^1 - V_{nn} \right] \tag{24.1}$$

$$0 = (\text{quartic}) \left\{ -E_n^2 - \sum_i \frac{V_{ni}V_{in}}{D_{in}} - \left[E_n^1 - V_{nn} \right] \sum_i \frac{V_{ii}}{D_{in}} \right\} + (\text{cubic}) E_n^1 \left[E_n^1 - V_{nn} \right]$$
(24.2)

$$0 = (\text{quartic}) \left\{ -E_n^3 + \sum_{ij} \frac{V_{ni} V_{ij} V_{jn}}{D_{in} D_{jn}} - E_n^1 \sum_i \frac{V_{ni} V_{in}}{D_{in} D_{in}} - \left[E_n^2 + \sum_i \frac{V_{ni} V_{in}}{D_{in}} \right] \sum_k \frac{V_{kk}}{D_{kn}} - \left[E_n^1 - V_{nn} \right] \left(E_n^1 \sum_k \frac{V_{kk}}{D_{kn} D_{kn}} - \frac{1}{2} \sum_{ij} \frac{V_{ij} V_{ji} - V_{ii} V_{jj}}{D_{in} D_{jn}} \right) \right\} + (\text{cubic}) \left\{ \left[E_n^2 + \sum_i \frac{V_{ni} V_{in}}{D_{in}} \right] E_n^1 + \left[E_n^1 - V_{nn} \right] \left(E_n^2 + E_n^1 \sum_i \frac{V_{ii}}{D_{in}} \right) \right\} - (\text{quadratic}) \left\{ \left[E_n^1 - V_{nn} \right] (E_n^1)^2 \right\}$$

0 =expressions of ascending order and complexity

<u>These equations comprise—in the non-degenerate case—the principal fruit</u> of the present formalism. We see that (24.1) is, in effect, a description of E_n^1 , and sends simplifications rippling downstream ... with the result that (24.2) becomes simply a description of E_n^2 , and dispatches further simplifications; (24.3) becomes a description of E_n^3 , etc. Were I interested in E_n^4 I would sidestep the heavy computation that goes into the demonstration that

$$\boxed{\text{STUFF}}_{4,1} = \boxed{\text{STUFF}}_{4,2} = \boxed{\text{STUFF}}_{4,3} = 0$$

and concentrate quartic component of $\fbox{GOOD STUFF}_4$. A vast amount of computational labor would thus be avoided.¹⁶

But if the unperturbed eigenvalue E_n is degenerate then (24.1) collapses into uninformative triviality, and the the downstream quartic terms—which a moment ago bore the full burden—all disappear. The burden of supplying information about E_n^1, E_n^2, \ldots falls to terms which in the non-degenerate case were found to be quiescent. I turn now to discussion of how this comes about.

Management of spectral degeneracy. In degenerate cases the perturbation theory of Rayleigh-Schrödinger tends (in my eccentric view) to degenerate into an off-putting mess. I for a while entertained the hope that the present formalism—because it obviates any need to be concerned with perturbed eigen*vectors*—would in this problem area present distinct advantages. It does not: the best that can be said is that it presents us with a (somewhat) *different* mess.

An instance of the line of argument to which the present formalism gives rise was encountered already when the 2-state theory led us to (10); here I undertake to enlarge upon the lesson of that example. In an effort to keep simple things simple I make use once again of the explicit language that becomes available when one assumes state space to be 5-dimensional.

Let us for the moment assume that the unperturbed spectrum, which had formerly the design $\{E_1, E_2, E_3, E_4, E_n\}$, has assumed the singly-degenerate design

 $\{E_1, E_2, E_3, E_m, E_n\}$ with $E_m = E_n$

Then D_{mn} (formerly written D_{4n}) vanishes, which kills all previous "quartic" factors; kills also some of the terms which formerly contributed to the definitions of "cubic," "quadratic," "linear;" and introduces a singularity into all previous summands. Those circumstances, as will emerge, cause information to shift about—to "percolate"—amongst the terms in preceding expressions, and some new information to come to rest in terms called <u>NEW GOOD STUFF</u>. The death of "quartic" means (as will soon become apparent) that control has been inherited by somebody named "new cubic," whom I now introduce:

¹⁶ Note added on 24 September 2000: Oz Bonfim has today informed me that (23.3) is presented as Problem 2 on page 136 of the 3^{rd} edition (1977) of Landau & Lifshitz' *Quantum Mechanics*. It does not appear in earlier editions.

Management of spectral degeneracy

Working from the top of p. 16, we find¹⁷

$$(quartic) \equiv D_{1n}D_{2n}D_{3n}D_{4n}$$

$$\downarrow$$

$$= D_{1n}D_{2n}D_{3n}D$$

$$\equiv (new \text{ cubic})D$$

$$(cubic) \equiv D_{1n}D_{2n}D_{3n} + D_{1n}D_{2n}D_{4n} + D_{1n}D_{3n}D_{4n}$$

$$\downarrow$$

$$= D_{1n}D_{2n}D_{3n} + D_{1n}D_{2n}D + D_{1n}D_{3n}D$$

$$\equiv (new \text{ cubic}) + (new \text{ quadratic})D$$

$$(quadratic) \equiv D_{1n}D_{2n} + D_{1n}D_{3n} + D_{2n}D_{3n} + D_{1n}D_{4n} + D_{2n}D_{4n} + D_{3n}D_{4n}$$

$$\downarrow$$

$$= D_{1n}D_{2n} + D_{1n}D_{3n} + D_{2n}D_{3n} + D_{1n}D_{4n} + D_{2n}D_{4n} + D_{3n}D_{4n}$$

$$\downarrow$$

$$= D_{1n}D_{2n} + D_{1n}D_{3n} + D_{2n}D_{3n} + D_{1n}D + D_{2n}D + D_{3n}D$$

$$\equiv (new \text{ quadratic}) + (new \text{ linear})D$$

where now all subscripts $_n$ could as well be written $_m$. Note, however, that this is *not* true when the subscripts decorate V.

Look to the 2nd-order consequences of these adjustments. Reading from pp. 16–17 we find (after omission of all final terms proportional to D = 0)

$$\begin{array}{l} \hline \text{FIRST TERM: SECOND ORDER} \\ \downarrow \\ (E_n^1)^2 \Big\{ (\text{new cubic} + (\text{new quadratic}) D \Big\} - E_n^2 (\text{new cubic}) D \\ = (\text{new cubic}) (E_n^1)^2 \\ \hline \text{SECOND TERM: SECOND ORDER} \\ \downarrow \\ = - \Big\{ E_n^1 (\text{new cubic}) D \Big[\sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{mm}}{D} \Big] + E_n^1 V_{nn} (\text{new cubic}) \Big\} \\ - E_n^1 V_{nn} \frac{(\text{new cubic}) D}{D} \\ = -(\text{new cubic}) \Big\{ E_n^1 V_{mm} + 2E_n^1 V_{nn} \Big\} \\ \hline \text{THIRD TERM: SECOND ORDER} \\ \downarrow \\ = V_{nn} (\text{new cubic}) D \Big[\sum_i \frac{V_{ii}}{D_{in}} + \frac{V_{mm}}{D} \Big] + \frac{1}{2} V_{nn} V_{nn} \frac{(\text{new cubic}) D}{D} \\ \hline \end{array}$$

= (new cubic) $\left(V_{mm}V_{nn} + \frac{1}{2}V_{nn}V_{nn}\right)$

¹⁷ In place of $D_{mm} = D_{nn}$ I will henceforth write simply D.

FOURTH TERM: SECOND ORDER \downarrow $= E_n^1 V_{nn} \frac{(\text{new cubic})D}{D}$ $= (\text{new cubic})E_n^1 V_{nn}$ FIFTH TERM: SECOND ORDER \downarrow $= -(\text{new cubic})D\left[\sum_{i} \frac{V_{ni}V_{in}}{D_{in}} + \frac{V_{nm}V_{mn}}{D}\right] - \frac{1}{2}V_{nn}V_{nn} \frac{(\text{new cubic})D}{D}$

$$= -(\text{new cubic})D\left[\sum_{i} \frac{V_{ni}V_{in}}{D_{in}} + \frac{V_{nm}V_{mn}}{D}\right] - \frac{1}{2}V_{nn}V_{nn}\frac{(\text{new cubic})D}{D}$$
$$= -(\text{new cubic})\left\{V_{nm}V_{mn} + \frac{1}{2}V_{nn}V_{nn}\right\}$$

Summing up the preceding expressions, we are led to write

$$0 = \sum \overline{\text{FIVE TERMS}}$$

= (new cubic) $\cdot \left\{ (E_n^1)^2 - (V_{mm} + V_{nn})E_n^1 + (V_{mm}V_{nn} - V_{mn}V_{nm}) \right\}$

But if, as we have assumed, "new cubic" $\neq 0$ this amounts simply to the assertion that

$$\det \begin{pmatrix} V_{mm} - E_n^1 & V_{mn} \\ V_{nm} & V_{nn} - E_n^1 \end{pmatrix} = 0$$
(25)

In the contrary case the 2nd-order equation (22.2) collapses into triviality and we must look farther downstream to obtain information about E_n^1 . For example, in cases of the type

$$\{E_1, E_2, E_\ell, E_m, E_n\}$$
 with $E_\ell = E_m = E_n$

we expect to obtain

$$\det \begin{pmatrix} V_{\ell\ell} - E_n^1 & V_{\ell m} & V_{\ell n} \\ V_{m\ell} & V_{mm} - E_n^1 & V_{mn} \\ V_{n\ell} & V_{nm} & V_{nn} - E_n^1 \end{pmatrix} = 0$$

We must look to at least $3^{\rm rd}$ -order to resolve the degeneracy if the roots of (25) are coincident (as may happen), while if they are distinct we must look to $3^{\rm rd}$ -order to obtain information about E_n^2 . The list of possible circumstances proliferates rapidly; I will pursue none of the details, since the *method* by which they would be pursued is by now clear.

Simplifying special assumptions

Two classes of simplifying special assumptions. From the hermiticity of $\mathbb V$ it follows in the most general case that

$$\mathbb{V} = (\text{real symmetric } \mathbb{S}) + (\text{imaginary antisymmetric } \mathbb{A})$$

We look to the class of cases in which S vanishes; i.e., in which

$$\mathbb{V}$$
 is antisymmetric : $\mathbb{V}^{\mathsf{T}} = -\mathbb{V}$

In such cases we have

$$\mathrm{tr}\mathbb{V}^p = 0 \quad : \quad p \text{ odd} \tag{26}$$

The antisymmetry of $\mathbb V$ does not imply antisymmetry of matrix

$$\mathbb{M} \equiv \mathbb{D}\mathbb{V}$$
 : $\mathbb{D} \equiv (\mathbb{H}^0 - E\mathbb{I})^{-1}$ is diagonal

introduced at (11). But (26) nevertheless persists

$$T_p \equiv \operatorname{tr} \mathbb{M}^p = 0 \quad : \quad p \text{ odd} \tag{27}$$

as a special instance of the following more general proposition: from symmetric \mathbb{S} and antisymmetric \mathbb{A} construct $[(\mathbb{S}\mathbb{A})^p]^{\mathsf{T}} = (-)^p \mathbb{A}(\mathbb{S}\mathbb{A})^{p-1}\mathbb{S}$, then use general properties of the trace¹⁸ to obtain $\operatorname{tr}(\mathbb{S}\mathbb{A})^p = (-)^p \operatorname{tr}(\mathbb{S}\mathbb{A})^p = 0$ if p is odd. At (13) we in antisymmetric cases have

$ T_1 $	T_2	T_3	T_4	T_5	T_6	()	T_2	0	T_4	0	$T_6 \mid$
1	T_1	T_2	T_3	T_4	T_5	1	_	0	T_2	0	T_4	0
0	2	T_1	T_2	T_3	T_4)	2	0	T_2	0	T_4
0	0	3	T_1	T_2	T_3	$ \rightarrow ($)	0	3	0	T_2	0
0	0	0	4	T_1	T_2)	0	0	4	0	T_2
0	0	0	0	5	T_1)	0	0	0	5	0

which causes fairly dramatic simplifications (see, for example, what happens to (16): evidently $\Delta_{\text{odd}} = 0$) to propagate throughout the theory. In place of (22) we have

$$0 = P_0$$

$$0 = P_1$$

$$0 = P_2 - \frac{1}{2}P_0T_{20}$$

$$0 = P_3 - \frac{1}{2}P_1T_{20} - \frac{1}{2}P_0T_{21}$$

$$\vdots$$

From (23.1) we learn that

If \mathbb{V} is antisymmetric then $E_n^1 = 0$: the leading spectral adjustment is of 2^{nd} order.

¹⁸ tr $\mathbb{X}^{\mathsf{T}} = \operatorname{tr} \mathbb{X}$ and tr $\mathbb{X}\mathbb{Y} = \operatorname{tr} \mathbb{Y}\mathbb{X}$.

This last circumstance brings to mind some aspects of the quantum theory of the Stark effect, but the cleanest example of a system with "antisymmetric perturbation" is provided by the perturbed harmonic oscillator:

$$\mathbf{H} = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}m\omega^2\mathbf{x}^2 + \lambda\sqrt{\frac{2\hbar\omega}{m}}\mathbf{p}$$

since relative to the unperturbed oscillator eigenbasis $\{|n\}$ one has¹⁹

$$\|(m|\mathbf{p}|n)\| = i\sqrt{m\hbar\omega/2} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & \ddots \\ +\sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & \ddots \\ 0 & +\sqrt{2} & 0 & -\sqrt{3} & 0 & \ddots \\ 0 & 0 & +\sqrt{3} & 0 & -\sqrt{4} & \ddots \\ 0 & 0 & 0 & +\sqrt{4} & 0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

Even more dramatic are the simplifications which result when ${\sf V}$ possesses the projective form

$$\mathbf{V} = |V)(V| \tag{28}$$

characteristic of what is called "pair theory." $^{20}\,$ For then a simple argument gives

$$\operatorname{tr} \mathbb{M}^{p} = (\operatorname{tr} \mathbb{M})^{p}$$
$$\operatorname{tr} \mathbb{M} = \sum_{m,n} (m | (\mathbf{H}^{0} - E \mathbf{I})^{-1} | n) (n | V) (V | m) = \sum_{n} \frac{|(n | V)|^{2}}{E_{n} - E}$$

so we have

$$det(\mathbb{I} + \lambda \mathbb{M}) = e^{\operatorname{tr} \log(\mathbb{I} + \lambda \mathbb{M})}$$
$$= e^{\log(1 + \lambda \operatorname{tr} \mathbb{M})}$$
$$= 1 + \lambda \sum_{n} \frac{|(n|V)|^2}{E_n - E}$$

Our problem, therefore, is to locate the zeros of

$$f(E) \equiv \left\{ 1 + \lambda \sum_{i} \frac{|(i|V)|^2}{E_i - E} \right\} \cdot \prod_{j} (E_j - E)$$

¹⁹ See, for example, A. Massian, *Quantum Mechanics* (1966), Chapter 12, §5.

 $^{^{20}}$ E. M. Henley & W. Thirring devote Chapters 11 & 12 of their *Elementary Quantum Field Theory* (1962) to this subject (which I have stripped to the bare bones), and give references to the physical literature. The subject is treated also on pp. 21–30 in my QUANTUM PERTURBATIONS.³

Conclusions & prospects

This we would do by expanding $f(E_n + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots)$ as an explicit power series in λ and then undertaking to solve serially the equations that result from setting the coefficients equal to zero. I have developed the details elsewhere, so will not repeat them here. This much, however, is clear: the computational program that ensues is a great deal simpler than the program—developed in these pages—to which one is committed when the condition (28) is absent.

Concluding remarks and prospects. The preceding material sprang from a seed accidentally turned up by my plow while preparing some recent "lectures on advanced quantum mechanics." On the last day of class I returned to the topic in the naive expectation that a write-up might run to six or eight pages. That "naive expectation" was based on the—mistaken—thought that "perturbation theory is a simple subject, made traditionally more complicated than it need be by a computational scheme that requires one to answer questions one had not intended to ask." I come away with the impression that perturbation theory is in fact a subject of *intrinsic* complexity: labor to make it simple in this respect, and it becomes complicated in that one. One can say simple things complicated things simply.

To the critic who objects that I have constructed a mere tour de force and that to no real purpose—I have no very convincing response. For (i) data seldom supports an interest in high-order perturbation theory, and (ii) if it did, people would by now (by whatever means) have developed the relevant formulæ and written them down in books, there to be consulted as needed (no need to perpetually *rederive* such formulæ). Besides, the heavy labor is associated not so much with the production of formulæ as with the exact/approximate description of the matrix elements that must, in each physical instance, be inserted into them, and with the evaluation of the resulting sums. It is, I have to admit, a little bit precious to be concerned (as I have been) exclusively with the production of formulæ, and not at all with their practical use.

Yet it does seem to me to be of *methodological* interest—and potentially of relevance to work having nothing at all to do with perturbation theory—that we have been able

- construct a workable theory of ∞ -dimensional determinants;
- say things about the roots of a "polynomial" of infinite order;
- develop a theory of perturbed spectra that avoids all reference to perturbed states.

I have been working things out as I went along, and could not have done the work without the cut/paste resources of Textures (the Blue Sky Research implementation of T_EX). I presume of my reader that he/she has the good sense to skip the overwhelming detail, which I have allowed to remain for one reason: the whole theory has a distinctly "algorithmic" quality, and all the labor should ideally be assigned to a computer. I have been writing with an eye to the needs of the student who I hope one day will undertake that project.