Time-independent perturbation theory by

BRACCI'S METHOD

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Spring 2007

Introduction

Let E_n denote the eigenvalues, and $|n)$ the orthonormal eigenvectors (both of which we assume to be known), of the unperturbed Hamiltonian $\mathbf{H}$:

$$\mathbf{H}|n) = E_n|n)$$

Assume the spectrum of $\mathbf{H}$ to be non-degenerate. We seek to describe perturbed eigenvalues $E_n + \lambda X_1 + \lambda^2 X_2 + \lambda^3 X_3 \cdots$ of the perturbed Hamiltonian $\mathbf{H} + \lambda\mathbf{V}$.

Writing $|n) + \lambda|\phi_1) + \lambda^2|\phi_2) + \lambda^3|\phi_3) + \cdots$ to describe the (un-normalized) perturbed eigenvector, we have

$$\begin{aligned}(\mathbf{H} + \lambda\mathbf{V})&[\,|n) + \lambda|\phi_1) + \lambda^2|\phi_2) + \lambda^3|\phi_3) + \cdots]\\ &= (E_n + \lambda X_1 + \lambda^2 X_2 + \lambda^3 X_3 \cdots)[\,|n) + \lambda|\phi_1) + \lambda^2|\phi_2) + \lambda^3|\phi_3) + \cdots]\end{aligned}$$

we have

$$\begin{aligned}\mathbf{H}|n) &= E_n|n)\\ \mathbf{H}|\phi_1) + \mathbf{V}|n) &= |\phi_1)E_n + |n)X_1\\ \mathbf{H}|\phi_2) + \mathbf{V}|\phi_1) &= |\phi_2)E_n + |\phi_1)X_1 + |n)X_2\\ \mathbf{H}|\phi_3) + \mathbf{V}|\phi_2) &= |\phi_3)E_n + |\phi_2)X_1 + |\phi_1)X_2 + |n)X_3\\ &\vdots\\ \mathbf{H}|\phi_p) + \mathbf{V}|\phi_{p-1}) &= |\phi_p)E_n + \sum_{k=1}^{p-1}|\phi_{p-k})X_k + |n)X_p \qquad (1)\end{aligned}$$

Multiplying (1) by $(n|$ we get

$$E_n(n|\phi_p) + (n|\mathbf{V}|\phi_{p-1}) = \Big\{(n|\phi_p)E_n + \sum_{k=1}^{p-1}(n|\phi_{p-k})X_k\Big\} + (n|n)X_p$$

which after slight simplification/rearrangement becomes

$$X_p = (n|\mathbf{V}|\phi_{p-1}) - \sum_{k=1}^{p-1}(n|\phi_{p-k})X_k \quad : \quad p \geqslant 2 \qquad (2)$$

—the leading instances of which read

$$
\begin{aligned}
X_1 &= (n|\mathbf{V}|n)\\
X_2 &= (n|\mathbf{V}|\phi_1) - (n|\phi_1)X_1\\
X_3 &= (n|\mathbf{V}|\phi_2) - (n|\phi_2)X_1 - (n|\phi_1)X_2\\
X_4 &= (n|\mathbf{V}|\phi_3) - (n|\phi_3)X_1 - (n|\phi_2)X_2 - (n|\phi_1)X_3\\
&\ \,\vdots
\end{aligned}
$$

Drawing upon the completeness relation

$$\sum_m |m)(m| = |n)(n| + \sum_{i\neq n} |i)(i| = \mathbf{I}$$

we have

$$(n|\mathbf{V}|\phi) = V_{nn}(n|\phi) + \sum_{i\neq n} V_{ni}(i|\phi)$$

and the preceding equations become

$$X_1 = V_{nn} \tag{2.1}$$

$$X_2 = V_{nn}(n|\phi_1) + \sum_{i\neq n} V_{ni}(i|\phi_1) - (n|\phi_1)X_1 \tag{2.2}$$

$$X_3 = V_{nn}(n|\phi_2) + \sum_{i\neq n} V_{ni}(i|\phi_2) - (n|\phi_2)X_1 - (n|\phi_1)X_2 \tag{2.3}$$

$$X_4 = V_{nn}(n|\phi_3) + \sum_{i\neq n} V_{ni}(i|\phi_3) - (n|\phi_3)X_1 - (n|\phi_2)X_2 - (n|\phi_1)X_3 \tag{2.4}$$

$$\vdots$$

Now multiply (1) by $(i\,| \neq (n|$ to obtain

$$E_i(i\,|\phi_p) + (i\,|\mathbf{V}|\phi_{p-1}) = \Big\{(i\,|\phi_p)E_n + \sum_{k=1}^{p-1}(i\,|\phi_{p-k})X_k\Big\}$$

or

$$(i\,|\phi_p) = D_{in}^{-1}\Big\{-(i\,|\mathbf{V}|\phi_{p-1}) + \sum_{k=1}^{p-1}(i\,|\phi_{p-k})X_k\Big\} \tag{3}$$

$$D_{in} \equiv E_i - E_n$$

—the leading instances of which read

$$(i\,|\phi_1) = D_{in}^{-1}\Big\{-(i\,|\mathbf{V}|n)\Big\} \quad : \quad \text{we have used } |\phi_0) \equiv |n) \tag{3.1}$$

$$(i\,|\phi_2) = D_{in}^{-1}\Big\{-(i\,|\mathbf{V}|\phi_1) + (i\,|\phi_1)X_1\Big\} \tag{3.2}$$

$$(i\,|\phi_3) = D_{in}^{-1}\Big\{-(i\,|\mathbf{V}|\phi_2) + (i\,|\phi_2)X_1 + (i\,|\phi_1)X_2\Big\} \tag{3.3}$$

$$(i\,|\phi_4) = D_{in}^{-1}\Big\{-(i\,|\mathbf{V}|\phi_3) + (i\,|\phi_3)X_1 + (i\,|\phi_2)X_2 + (i\,|\phi_1)X_3\Big\} \tag{3.4}$$

$$\vdots$$

in connection with which we have (as was already noted in the case $i = n$)

$$(i\,|\mathbf{V}|\phi) = V_{ii}(i\,|\phi) + \sum_{j\neq i} V_{ij}(j|\phi) \tag{4}$$

Bracci's method

Luciano Bracci makes essential use of the fact—stressed long ago by Saul Epstein (AJP**22**, 613 (1954) and AJP **36**, 165 (1968))—that one can without loss of generality always assume (or arrange for it to be the case) that

$$(n|\phi_1) = (n|\phi_2) = \cdots = 0 \tag{5}$$

Equations (2) then assume the simple form

$$\begin{aligned}
X_1 &= V_{nn} && (6.1)\\
X_2 &= V_{ni}G_{i1} && (6.2)\\
X_3 &= V_{ni}G_{i2} && (6.3)\\
X_4 &= V_{ni}G_{i3} && (6.4)\\
&\vdots
\end{aligned}$$

where by (3)

$$\begin{aligned}
G_{i1} &= -W_{in}V_{in} && (7.1)\\
G_{i2} &= -W_{in}(i\,|\mathbf{V}|\phi_1) + W_{in}\Big\{X_1G_{i1}\Big\} && (7.2)\\
G_{i3} &= -W_{in}(i\,|\mathbf{V}|\phi_2) + W_{in}\Big\{X_1G_{i2} + X_2G_{i1}\Big\} && (7.3)\\
G_{i4} &= -W_{in}(i\,|\mathbf{V}|\phi_3) + W_{in}\Big\{X_1G_{i3} + X_2G_{i2} + +X_3G_{i1}\Big\} && (7.3)\\
&\vdots
\end{aligned}$$

Here $\sum_{i\neq n}$ symbols have been surpressed,

$$W_{in} \equiv D_{in}^{-1} \equiv (E_i - E_n)^{-1}$$

and—by appeal simultaneously to the completeness relation and to (6)—

$$\begin{aligned}
(i\,|\mathbf{V}|n) &= V_{in}\\
(i\,|\mathbf{V}|\phi_1) &= V_{ij}G_{j1}\\
(i\,|\mathbf{V}|\phi_2) &= V_{ij}G_{j2}\\
(i\,|\mathbf{V}|\phi_3) &= V_{ij}G_{j3}\\
&\vdots
\end{aligned}$$

Feeding this information into (7) we obtain

$$G_{i1} = -W_{in}V_{in} \tag{8.1}$$

$$G_{i2} = -W_{in}V_{ij}G_{j1} + W_{in}\Big\{X_1G_{i1}\Big\} \tag{8.2}$$

$$G_{i3} = -W_{in}V_{ij}G_{j2} + W_{in}\Big\{X_1G_{i2} + X_2G_{i1}\Big\} \tag{8.3}$$

$$G_{i4} = -W_{in}V_{ij}G_{j3} + W_{in}\Big\{X_1G_{i3} + X_2G_{i2} + X_3G_{i1}\Big\} \qquad (8.3)$$

$$\vdots$$

It is by feeding equations (8) recursively into equations (6) that Bracci and his collaborators undertake to construct descriptions of $X_p : p = 2, 3, \ldots$ I look to leading examples of his procedure:

$$\begin{aligned} X_2 &= V_{ni}G_{i1} \\ &= V_{ni}\big[-W_{in}V_{in}\big] \\ &= -\frac{V_{ni}V_{in}}{D_{in}} \end{aligned}$$

$$\begin{aligned} X_3 &= V_{ni}G_{i2} \\ &= V_{ni}\big\{-W_{in}(i\,|\mathbf{V}|\phi_1) + W_{in}X_1G_{i1}\big\} \\ &= V_{ni}\big\{-W_{in}V_{ij}G_{j1} + W_{in}X_1G_{i1}\big\} \\ &= V_{ni}\big\{-W_{in}V_{ij}\big[-W_{jn}V_{jn}\big] + W_{in}X_1\big[-W_{in}V_{in}\big]\big\} \\ &= \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}} - X_1\frac{V_{ni}V_{in}}{D_{in}^2} \\ &= \frac{V_{ni}V_{ij}V_{jn}}{D_{in}D_{jn}} - V_{nn}\frac{V_{ni}V_{in}}{D_{in}^2} \end{aligned}$$

I found it exasperating to try to carry such hand calculation to higher order (though Bracci himself seems to manage very well). But in an accompanying notebook I show how *Mathematica* can be conscripted to carry such calculations to high order very quickly and efficiently, with very little labor.

Construction of perturbed eigenstates

The perturbation sends

$$\begin{aligned} |n) \longmapsto &\mathcal{N}\big\{|n) + \lambda|\phi_1) + \lambda^2|\phi_2) + \lambda^3|\phi_3) + \cdots\big\} \\ =&\mathcal{N}\big\{|n) + \sum_{i\neq n}\lambda|i)(i\,|\phi_1) + \lambda^2|i)(i\,|\phi_2) + \lambda^3|i)(i\,|\phi_3) + \cdots\big\} \\ =&\mathcal{N}\big\{|n) + \sum_{i\neq n}|i)\big[\lambda G_{i1} + \lambda^2G_{i2} + \lambda^3G_{i3} + \cdots\big]\big\} \qquad (9) \\ (n| \longmapsto &\mathcal{N}\big\{(n| + \sum_{i\neq n}(i|\big[\lambda\bar{G}_{i1} + \lambda^2\bar{G}_{i2} + \lambda^3\bar{G}_{i3} + \cdots\big]\big\} \end{aligned}$$

where $\mathcal{N}$ is a normalization factor:

$$\begin{aligned}\mathcal{N} &= \Big[1+\sum_{i\neq n}\big|\big[\lambda G_{i1}+\lambda^2 G_{i2}+\lambda^3 G_{i3}+\cdots\big]\big|^2\Big]^{\frac{1}{2}}\\ &= 1+\lambda^1\mathcal{N}_1+\lambda^2\mathcal{N}_2+\lambda^3\mathcal{N}_3+\cdots\end{aligned}$$

Though $\mathcal{N}_1 = 0$, the expressions that describe $\mathcal{N}_p = 0$ $(p \geqslant 2)$ are unavoidably very complicated. And so also, therefore, are the expressions $|\psi_{nk})$ that when inserted into

$$|n) \longmapsto |n) + \lambda^1|\psi_{n1}) + \lambda^3|\psi_{n3}) + \lambda^3|\psi_{n3}) + \cdots$$

serve to describe the perturbed eigenfunctions. It is, therefore, of perhaps only academic interest to notice that once one has acquired—whether by Bracci's method or mine—descriptions of $\{X_1, X_2, X_3, \ldots\}$ then one can use (8) to obtain recursive evaluations of $\{G_{i1}, G_{i2}, G_{i3}, \ldots\}$, whereupon it becomes possible in principle "simply to write down" descriptions of the perturbed eigenvectors, without further calculation.

Epstein's contribution It is, as Bracci observes, "well known that [perturbative] corrections $X_{n,p}$ to the energy [eigenvalues E_n] are independent of the components $(n|\phi_{n,p})$ of the perturbative corrections to the wave function," in which connection he cites Saul T. Epstein, "Uniqueness of the energy in perturbation theory," AJP **36**, 165 (1968). It was "by reversing that observation" that Bracci was led to his method: instead of looking to (1) to *establish* that the $X_{n,p}$ are independent of the $(n|\phi_{n,q})$ $(q = 1, 2, \ldots, p-1)$ he cleverly *insists* upon that independence, and is led promptly to his results. Actually, the point upon which Bracci insists was established very elegantly in an earlier Epstein paper ("Note on perturbation theory," AJP **22**, 613 (1954)). But Epstein's primary objective in that early paper was to describe a relatively slight improvement upon the clumsy Rayleigh-Schrödinger formalism that is standard to the textbooks—a formalism with which it is, in practice, virtually impossible to obtain spectral perturbations of high order.