Time-Independent Perturbation Theory

Robert Gilmore
Physics Department, Drexel University, Philadelphia, Pennsylvania 19104, USA

(Dated: January 30, 2007, *My Physics Class*: Quantum Mechanics I)

Perturbation theory is introduced by diagonalizing a 3×3 matrix. Generalization to a larger basis is immediate. This treatment is simpler than the usual treatment and leads immediately to results one higher order than usual in both the perturbed eigenvalues and eigenfunctions.

I. INTRODUCTION

Computing eigenvalues/vectors is all about diagonalizing matrices: finite $\times$ finite or $\infty \times \infty$. We treat the problem

$$H_0 + \epsilon H_1 = \left[\begin{array}{c|c|c} E_1 I_a + * & * & * \\ \hline * & E_2 I_b + * & * \\ \hline * & * & * \end{array} \right] \tag{1}$$

If some eigenvalues of H_0 are degenerate (e.g., the $2p$ levels in hydrogen) then corresponding submatrices should first be diagonalized: for example $E_1 I_a + \epsilon (H_1)_{ij}$, where $(H_1)_{ij}$ is the submatrix of ϵH_1 in the subspace of states that have degenerate eigenvalue E_1 of H_0.

II. A SIMPLE PERTURBATION PROBLEM

The method we propose is valid for H_0 with nondegenerate eigenvalues. All the results we need can be determined by using a simple 3×3 matrix and then applying the rules of "general covariance" at the end of the calculation.

We want to compute the eigenvalues and eigenvectors of the 3×3 matrix $H_0 + \epsilon H_1$. We begin by constructing the secular equation from

$$\left[\begin{array}{ccc} E_1 + \epsilon h_{11} - \lambda & \epsilon h_{12} & \epsilon h_{13} \\ \epsilon h_{21} & E_2 + \epsilon h_{22} - \lambda & \epsilon h_{23} \\ \epsilon h_{31} & \epsilon h_{32} & E_3 + \epsilon h_{33} - \lambda \end{array} \right] \rightarrow$$

$$\begin{array}{c} (E_1 + \epsilon h_{11} - \lambda)(E_2 + \epsilon h_{22} - \lambda)(E_3 + \epsilon h_{33} - \lambda) \\ +\epsilon^3 (h_{23} h_{31} h_{12} + h_{21} h_{13} h_{32}) \\ -\epsilon^2 (E_1 + \epsilon h_{11} - \lambda) h_{23} h_{32} \\ -\epsilon^2 (E_2 + \epsilon h_{22} - \lambda) h_{31} h_{13} \\ -\epsilon^2 (E_3 + \epsilon h_{33} - \lambda) h_{12} h_{21} \end{array} \tag{2}$$

where $(\epsilon (H_1)_{ij} \rightarrow \epsilon h_{ij})$. To determine the eigenvalues we set the determinant equal to zero.

We shall solve for the perturbation of the eigenvalue E_2. To do this we set the determinant equal to zero, divide by $(E_1 + \epsilon h_{11} - \lambda)(E_3 + \epsilon h_{33} - \lambda)$, and rearrange the equation to find

$$(E_2 + \epsilon h_{22} - \lambda) = -A\epsilon^2 - B\epsilon^2 - C\epsilon^3 \tag{3}$$

so that

$$\lambda = E_2 + \epsilon h_{22} + \epsilon^2 (A + B) + \epsilon^3 C \tag{4}$$

The terms A, B, C in this expression are:

$$\begin{array}{rcl} A & = & -\dfrac{(E_2 + \epsilon h_{22} - \lambda) h_{31} h_{13}}{(E_1 + \epsilon h_{11} - \lambda)(E_3 + \epsilon h_{33} - \lambda)} \\ B & = & -\dfrac{h_{21} h_{12}}{(E_1 + \epsilon h_{11} - \lambda)} - \dfrac{h_{23} h_{32}}{(E_3 + \epsilon h_{33} - \lambda)} \\ C & = & \dfrac{h_{23} h_{31} h_{12} + h_{21} h_{13} h_{32}}{(E_1 + \epsilon h_{11} - \lambda)(E_3 + \epsilon h_{33} - \lambda)} \end{array} \tag{5}$$

The coefficients A, B, C are functions of ϵ. Since $\lambda - (E_2 + \epsilon h_{22})$ is of order ϵ^2 (c.f, Eq. (3)), the term $A\epsilon^2$ is fourth order and can be neglected if we wish to compute corrections to E_2 only to third order. The coefficients B and C have Taylor series in ϵ beginning with a constant term.

To construct the correction to the energy E_2 to third order it is sufficient to replace $\lambda \rightarrow E_2 + \epsilon h_{22}$ in the denominators of B and C. We find

$$\begin{array}{l} E_2^{(3)} = E_2 + \epsilon h_{22} + \epsilon^2 \displaystyle\sum_{j \neq 2}^{3} \frac{h_{2j} h_{j2}}{(E_2 - E_j) + \epsilon (h_{22} - h_{jj})} \\ \qquad + \epsilon^3 \displaystyle\sum_{j \neq 2, k}^{3} \sum_{k \neq 2}^{3} \frac{h_{2j} h_{jk} h_{k2}}{(E_2 - E_j)(E_2 - E_k)} \end{array} \tag{6}$$

TABLE I: Terms of order ϵ and ϵ^2 obtained by multiplying out the matrices in Eq. (10).

Index	Order 1	Order 2
1	$u_1(E_1 - E_2) + h_{12}$	$v_1(E_1 - E_2) + u_1(h_{11} - h_{22}) + h_{12}u_2 + h_{13}u_3$
2	–	$h_{21}u_1 + h_{23}u_3 - B(0)$
3	$u_3(E_3 - E_2) + h_{32}$	$v_3(E_3 - E_2) + u_3(H_{33} - h_{22}) + h_{31}u_1 + h_{32}u_2$

III. INCREASING THE BASIS

The result, to third order, valid for any H_0 with non-degenerate levels, and arbitrary H_1, is simply obtained by: $2 \to i$ and removing the limits 3 in the summations above ("Principle of General Covariance"):

$$\begin{aligned} E_i^{(3)} &= E_i + \epsilon h_{ii} + \epsilon^2 \sum_{j \neq i} \frac{h_{ij} h_{ji}}{(E_i - E_j) + \epsilon(h_{ii} - h_{jj})} \\ &+ \epsilon^3 \sum_{j \neq i,k} \sum_{k \neq i} \frac{h_{ij} h_{jk} h_{ki}}{(E_i - E_j)(E_i - E_k)} \end{aligned} \tag{7}$$

In the familiar Dirac form this is

$$\begin{aligned} E_i^{(3)} &= E_i + \langle i|\epsilon H_1|i\rangle + \sum_{j \neq i} \frac{\langle i|\epsilon H_1|j\rangle\langle j|\epsilon H_1|i\rangle}{E_i^{(1)} - E_j^{(1)}} \\ &+ \sum_{j \neq i,k} \sum_{k \neq i} \frac{\langle i|\epsilon H_1|j\rangle\langle j|\epsilon H_1|k\rangle\langle k|\epsilon H_1|i\rangle}{(E_i - E_j)(E_i - E_k)} \end{aligned} \tag{8}$$

In this expression $E_j^{(1)} = E_j + \langle j|\epsilon H_1|j\rangle$.

IV. WAVEFUNCTIONS

Expressions for the perturbed wavefunctions are obtained by similar methods. We first write down the eigenvector equation for a generic perturbed wavefunction to second order in the smallness parameter ϵ:

$$\begin{bmatrix} E_1 - E_2 + \epsilon(h_{11} - h_{22}) & \epsilon h_{12} & \epsilon h_{13} \\ \epsilon h_{21} & -B(0)\epsilon^2 & \epsilon h_{23} \\ \epsilon h_{31} & \epsilon h_{32} & E_3 - E_2 + \epsilon(h_{33} - h_{22}) \end{bmatrix} \times \begin{bmatrix} +\epsilon u_1 + \epsilon^2 v_1 \\ 1 + \epsilon u_2 + \epsilon^2 v_2 \\ +\epsilon u_3 + \epsilon^2 v_3 \end{bmatrix} = 0 \tag{9}$$

These two matrices are multiplied out. Terms of order ϵ and ϵ^2 are collected in Table 1.

The perturbed vector, to second order in ϵ, is

$$\begin{bmatrix} 0 - \epsilon\left(\frac{h_{12}}{E_1 - E_2}\right) + \epsilon^2 \left\{ + \frac{h_{12}(h_{11} - h_{22})}{(E_1 - E_2)^2} + \frac{h_{13}h_{32}}{(E_1 - E_2)(E_3 - E_2)} \right\} \\ 1 \\ 0 - \epsilon\left(\frac{h_{32}}{E_3 - E_2}\right) + \epsilon^2 \left\{ + \frac{h_{32}(h_{33} - h_{22})}{(E_3 - E_2)^2} + \frac{h_{31}h_{12}}{(E_3 - E_2)(E_1 - E_2)} \right\} \end{bmatrix} \tag{10}$$

From this result we can write down the general result by inspection and substitution:

$$\begin{aligned} |i\rangle(\epsilon) &= |i\rangle - \sum_{j \neq i} |j\rangle \frac{\langle j|\epsilon H_1|i\rangle}{E_j - E_i} \\ &+ \sum_{j \neq i} |j\rangle \frac{\langle j|\epsilon H_1|i\rangle(\langle j|\epsilon H_1|j\rangle - \langle i|\epsilon H_1|i\rangle)}{(E_j - E_i)^2} \\ &+ \sum_{j \neq k,i} \sum_{k \neq i} |j\rangle \frac{\langle j|\epsilon H_1|k\rangle\langle k|\epsilon H_1|i\rangle}{(E_j - E_i)(E_k - E_i)} \end{aligned} \tag{11}$$

This is the standard result in time-independent perturbation theory [1].

V. CONCLUSION

We have simplified the presentation of time-independent perturbation theory by presenting it for small 3×3 matrices, then extending in the obvious way to arbitrarily sized matrices.

ACKNOWLEDGMENTS

The author thanks several former classes for expressing disinterest in the standard presentations of this subject by falling asleep and snoring.

REFERENCES

[1] L. E. Ballentine, *Quantum Mechanics, A Modern Development*, Singapore: World Scientific, 1998.