# Time-Independent Perturbation Theory

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Perturbation theory is introduced by diagonalizing a $3 \times 3$ 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

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

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 $\epsilon H_1$ 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 $3 \times 3$ 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 $3 \times 3$ matrix $H_0 + \epsilon H_1$. We begin by constructing the secular equation from

$$\begin{bmatrix} E_1 + \epsilon h_{11} - \lambda & \epsilon h_{12} & \epsilon h_{13} \\ \epsilon h_{21} & E_2 + \epsilon h_{22} - \lambda & \epsilon h_{23} \\ \epsilon h_{31} & \epsilon h_{32} & E_3 + \epsilon h_{33} - \lambda \end{bmatrix} \rightarrow$$

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

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

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

so that

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

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

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

The coefficients $A, B, C$ are functions of $\epsilon$. Since $\lambda - (E_2 + \epsilon h_{22})$ is of order $\epsilon^2$ (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 $\epsilon$ 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

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

TABLE I: Terms of order $\epsilon$ and $\epsilon^2$ 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"):

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

In the familiar Dirac form this is

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

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 $\epsilon$:

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

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

The perturbed vector, to second order in $\epsilon$, 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:

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

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 $3 \times 3$ matrices, then extending in the obvious way to arbitrarily sized matrices.

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## REFERENCES

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