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

$$H_0 + \epsilon H_1 = \begin{bmatrix} E_1 I_a + \epsilon & \epsilon & \epsilon \\ \epsilon & E_2 I_b + \epsilon & \epsilon \\ \epsilon & \epsilon & E_3 + \epsilon \end{bmatrix}$$

(1)

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

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

(3)

so that

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

(4)

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

$$A = -\frac{(E_2 + \epsilon h_{22} - \lambda)h_{31}h_{13}}{(E_1 + \epsilon h_{11} - \lambda)(E_3 + \epsilon h_{33} - \lambda)}$$

$$B = -\frac{h_{31}h_{12}}{(E_1 + \epsilon h_{11} - \lambda)} - \frac{h_{23}h_{32}}{(E_3 + \epsilon h_{33} - \lambda)}$$

$$C = \frac{h_{23}h_{31}h_{12} + h_{21}h_{13}h_{32}}{(E_1 + \epsilon h_{11} - \lambda)(E_3 + \epsilon h_{33} - \lambda)}$$

(5)

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

$$E_2^{(3)} = E_2 + \epsilon h_{22} + \epsilon^2 \sum_{j \neq 2} \frac{h_{2j}h_{3j}}{(E_2 - E_j)(E_2 - E_k)} + \epsilon^3 \sum_{j \neq 2, k \neq 2} \frac{h_{2j}h_{jk}h_{k2}}{(E_2 - E_j)(E_2 - E_k)}$$

(6)
TABLE I: Terms of order $\epsilon$ and $\epsilon^2$ obtained by multiplying out the matrices in Eq. (10).

<table>
<thead>
<tr>
<th>Index</th>
<th>Order 1</th>
<th>Order 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$u_1(E_1 - E_2) + h_{12}$ $v_1(E_1 - E_2) + u_1(h_{11} - h_{22}) + h_{12}u_2 + h_{13}u_3$</td>
<td>$0 - \epsilon \left( \frac{h_{12}}{E_1 - E_2} \right) + \epsilon^2 \left{ \frac{h_{12}(h_{11} - h_{22})}{(E_1 - E_2)^2} + \frac{h_{13}h_{32}}{(E_1 - E_2)(E_3 - E_2)} \right}$</td>
</tr>
<tr>
<td>2</td>
<td>$- h_{21}u_1 + h_{23}u_3 - B(0)$</td>
<td>$1$</td>
</tr>
<tr>
<td>3</td>
<td>$u_3(E_3 - E_2) + h_{32}$ $v_3(E_3 - E_2) + u_3(H_{33} - h_{22}) + h_{31}u_1 + h_{32}u_2$</td>
<td>$0 - \epsilon \left( \frac{h_{32}}{E_3 - E_2} \right) + \epsilon^2 \left{ \frac{h_{32}(h_{33} - h_{22})}{(E_3 - E_2)^2} + \frac{h_{34}h_{42}}{(E_3 - E_2)(E_4 - E_2)} \right}$</td>
</tr>
</tbody>
</table>

### 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: $2 \rightarrow i$ and removing the limits 3 in the summations above (“Principle of General Covariance”):

$$E_i^{(3)} = E_i + \epsilon h_{ii} + \epsilon^2 \sum_{j \neq i} \frac{h_{ij}h_{ji}}{(E_i - E_j) + \epsilon(h_{ii} - h_{jj})}$$

$$+ \epsilon^3 \sum_{j \neq i} \sum_{k \neq i} \frac{h_{ij}h_{jk}h_{ki}}{(E_i - E_j)(E_j - E_k)}$$

(7)

In the familiar Dirac form this is

$$E_i^{(3)} = E_i + \langle i|\epsilon H_1|i \rangle + \sum_{j \neq i} \frac{\langle i|\epsilon H_1|j \rangle \langle j|\epsilon H_1|i \rangle}{E_i - E_j}$$

$$+ \sum_{j \neq k \neq i} \frac{\langle i|\epsilon H_1|j \rangle \langle j|\epsilon H_1|k \rangle \langle k|\epsilon H_1|i \rangle}{(E_i - E_j)(E_j - E_k)}$$

(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 $\epsilon$:

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

(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

$$0 - \epsilon \left( \frac{h_{12}}{E_1 - E_2} \right) + \epsilon^2 \left\{ \frac{h_{12}(h_{11} - h_{22})}{(E_1 - E_2)^2} + \frac{h_{13}h_{32}}{(E_1 - E_2)(E_3 - E_2)} \right\}$$

$$1$$

$$0 - \epsilon \left( \frac{h_{32}}{E_3 - E_2} \right) + \epsilon^2 \left\{ \frac{h_{32}(h_{33} - h_{22})}{(E_3 - E_2)^2} + \frac{h_{34}h_{42}}{(E_3 - E_2)(E_4 - E_2)} \right\}$$

(10)

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

$$|i\rangle (\epsilon) = |i\rangle - \sum_{j \neq i} \frac{|j\rangle \langle j|\epsilon H_1|i \rangle}{E_j - E_i}$$

$$+ \sum_{j \neq k \neq i} \frac{|j\rangle \langle j|\epsilon H_1|k \rangle \langle k|\epsilon H_1|i \rangle}{(E_j - E_i)(E_k - E_i)}$$

(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.

### ACKNOWLEDGMENTS

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

### REFERENCES