DEGENERATE PERTURBATION IN 3 STATE SYSTEM

Here's another example of multiple degenerate perturbation theory. This time, the system has only 3 linearly independent states, with the Hamiltonian given by

\[ H = V_0 \begin{bmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{bmatrix} \]  

(1)

where \( \epsilon \ll 1 \) and can be regarded as a perturbation. The unperturbed Hamiltonian is then

\[ H = V_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \]  

(2)

and has one state with energy \( 2V_0 \) and a two-fold degenerate state with energy \( V_0 \). The normalized eigenvectors are

\[
\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}
\]  

(3)

In this case, we can solve the perturbed system exactly by finding the eigenvalues of the full matrix from the equation

\[(1 - \epsilon - \lambda) [(1 - \lambda)(2 - \lambda) - \epsilon^2] = 0 \]  

(4)

The solutions of this equation are

\[
\lambda = \begin{cases} 
1 - \epsilon \\
\frac{3}{2} + \frac{1}{2}\sqrt{1 + 4\epsilon^2} \\
\frac{3}{2} - \frac{1}{2}\sqrt{1 + 4\epsilon^2}
\end{cases}
\]  

(5)

so the three energies are \( V_0\lambda \). We can expand the square root in the last two
energies in a Taylor series in $\epsilon^2$ using $\sqrt{1 + 4\epsilon^2} = 1 + 2\epsilon^2 + \mathcal{O}(\epsilon^4)$ so we get

$$E_\epsilon = \begin{cases} V_0 (1 - \epsilon) \\ V_0 \left( 2 + \epsilon^2 + \mathcal{O}(\epsilon^4) \right) \\ V_0 \left( 1 - \epsilon^2 + \mathcal{O}(\epsilon^4) \right) \end{cases} \tag{6}$$

We can see that two of these energies are perturbations on the original degenerate state with $E_0 = V_0$ and the third is a perturbation on $E_0 = 2V_0$.

We can now analyze the system using perturbation theory and compare the results with the exact solutions above. The perturbation is

$$V = V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \tag{7}$$

Since the unperturbed state with $E_0 = 2V_0$ is non-degenerate, we can use non-degenerate perturbation theory to find the change in energy. The state corresponding to this energy is given by the eigenvector $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, so the energy perturbation is given by

$$E_1 = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0 \tag{8}$$

This is consistent with the result above, since there is no first order term in $V_0 \left( 2 + \epsilon^2 + \mathcal{O}(\epsilon^4) \right)$. We can work out the second order correction using our earlier formula:

$$E_{n2} = \sum_{j \neq n} \frac{| \langle j0 | V | n0 \rangle |^2}{E_{n0} - E_{j0}} \tag{9}$$

For this, we need the off-diagonal matrix elements. If we number the eigenvectors of the unperturbed system above in order, then the $E_0 = 2$ state has $n = 3$, so we need

$$\langle 20 | V | 30 \rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \epsilon V_0 \tag{10}$$

$$\langle 10 | V | 30 \rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} V_0 \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0 \tag{11}$$
Since \( E_{3,0} - E_{j,0} = V_0 \) for \( j = 1,2 \) we get

\[
E_{3,2} = \frac{|\langle 20|V|30 \rangle|^2}{V_0} = V_0 \epsilon^2
\]  

(12)

This correction term matches the \( \epsilon^2 \) term in the expansion above: \( V_0 \left( 2 + \epsilon^2 + O(\epsilon^4) \right) \).

For the degenerate energy \( E_0 = V_0 \), we can use degenerate perturbation theory, but only up to first order since we haven’t worked out the higher order cases. In this case, the matrix \( W \) is a 2 \( \times \) 2 matrix, since the unperturbed state is only doubly degenerate. We get

\[
W_{11} = \langle 10|V|10 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = -\epsilon V_0
\]  

(13)

\[
W_{21} = W_{12} = \langle 10|V|20 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0
\]  

(14)

\[
W_{22} = \langle 20|V|20 \rangle = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0
\]  

(15)

\[
W = \begin{bmatrix} -\epsilon V_0 & 0 \\ 0 & 0 \end{bmatrix}
\]  

(16)

Thus, to first order, one state gets an adjustment to the energy of \(-\epsilon V_0\) and the other gets zero, which is consistent with the exact results above, since there is no first order term in \( V_0 \left( 1 - \epsilon^2 + O(\epsilon^4) \right) \). Since \( W \) is diagonal, the special states are just the original states.