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

\[
H = V_0 \begin{bmatrix}
1 & -\epsilon_0 & 0 \\
0 & 1 & \epsilon \\
0 & \epsilon_0 & 2
\end{bmatrix}
\]  

(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

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

(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

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

(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 \( \sqrt{1 + 4\epsilon^2} = 1 + 2\epsilon^2 + O(\epsilon^4) \) so we get
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\[ E_\epsilon = \begin{cases} 
V_0 (1 - \epsilon) \\
V_0 (2 + \epsilon^2 + O(\epsilon^4)) \\
V_0 (1 - \epsilon^2 + O(\epsilon^4)) 
\end{cases} \quad (6) \]

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

\[ V = V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\
0 & 0 & \epsilon \\
0 & \epsilon & 0 \end{bmatrix} \quad (7) \]

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 \( \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \), so the energy perturbation is given by

\[ E_1 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\
0 & 0 & \epsilon \\
0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0 \quad (8) \]

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

\[ E_{n2} = \sum_{j \neq n} \frac{|\langle j | V | n \rangle|^2}{E_{n0} - E_{j0}} \quad (9) \]

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

\[ \langle 20 | V | 30 \rangle = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\
0 & 0 & \epsilon \\
0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \epsilon V_0 \quad (10) \]

\[ \langle 10 | V | 30 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\epsilon & 0 & 0 \\
0 & 0 & \epsilon \\
0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0 \quad (11) \]

Since \( E_{3,0} - E_{j,0} = V_0 \) for \( j = 1, 2 \) we get
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\[ E_{3,2} = \left| \frac{\langle 20 | V | 30 \rangle}{V_0} \right|^2 = V_0 \epsilon^2 \]  \hspace{1cm} (12)

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

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

\[
W_{11} = \langle 10 | V | 10 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} \epsilon^2 & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = -\epsilon V_0 \hspace{1cm} (13)
\]

\[
W_{21} = W_{12} = \langle 10 | V | 20 \rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} \epsilon^2 & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0 \hspace{1cm} (14)
\]

\[
W_{22} = \langle 20 | V | 20 \rangle = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} V_0 \begin{bmatrix} \epsilon^2 & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0 \hspace{1cm} (15)
\]

\[
W = \begin{bmatrix} -\epsilon V_0 & 0 \\ 0 & 0 \end{bmatrix} \hspace{1cm} (16)
\]

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 \( V_0 \left( 1 - \epsilon^2 + \mathcal{O} (\epsilon^4) \right) \). Since \( W \) is diagonal, the special states are just the original states.