DEGENERATE PERTURBATION IN 3 STATE SYSTEM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.9.

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

$$H = V_0 \begin{bmatrix} 1-\varepsilon & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{bmatrix} \tag{0.1}$$

where $\varepsilon \ll 1$ and can be regarded as a perturbation. The unperturbed hamiltonian is then

$$H = V_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \tag{0.2}$$

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

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{0.3}$$

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

$$(1-\varepsilon-\lambda)\left[(1-\lambda)(2-\lambda)-\varepsilon^2\right] = 0 \tag{0.4}$$

The solutions of this equation are

$$\lambda = \begin{cases} 1-\varepsilon \\ \frac{3}{2}+\frac{1}{2}\sqrt{1+4\varepsilon^2} \\ \frac{3}{2}-\frac{1}{2}\sqrt{1+4\varepsilon^2} \end{cases} \tag{0.5}$$

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

$$E_\varepsilon = \begin{cases} V_0\left(1-\varepsilon\right) \\ V_0\left(2+\varepsilon^2+\mathscr{O}\left(\varepsilon^4\right)\right) \\ V_0\left(1-\varepsilon^2+\mathscr{O}\left(\varepsilon^4\right)\right) \end{cases} \tag{0.6}$$

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

$$V = V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \tag{0.7}$$

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

$$E_1 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0 \tag{0.8}$$

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

$$E_{n2} = \sum_{j\neq n} \frac{\left|\langle j0|\, V\, |n0\rangle\right|^2}{E_{n0}-E_{j0}} \tag{0.9}$$

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

$$\langle 20|V|30\rangle = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \varepsilon V_0 \tag{0.10}$$

$$\langle 10|V|30\rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 0 \tag{0.11}$$

Since $E_{3,0} - E_{j,0} = V_0$ for $j = 1,2$ we get

$$E_{3,2} = \frac{|\langle 20|V|30\rangle|^2}{V_0} = V_0 \varepsilon^2 \tag{0.12}$$

This correction term matches the ε^2 term in the expansion above: $V_0\left(2+\varepsilon^2+\mathscr{O}\left(\varepsilon^4\right)\right)$.

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 2×2 matrix, since the unperturbed state is only doubly degenerate. We get

$$W_{11} = \langle 10|V|10\rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = -\varepsilon V_0 \tag{0.13}$$

(0.14)

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

$$W_{22} = \langle 20|V|20\rangle = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix} V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0 \tag{0.15}$$

$$W = \begin{bmatrix} -\varepsilon V_0 & 0 \\ 0 & 0 \end{bmatrix} \tag{0.16}$$

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