

## 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

$$H = V_0 \begin{bmatrix} 1 - \varepsilon & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{bmatrix} \quad (1)$$

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

$$H = V_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad (2)$$

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

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad (3)$$

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

$$(1 - \varepsilon - \lambda) [(1 - \lambda)(2 - \lambda) - \varepsilon^2] = 0 \quad (4)$$

The solutions of this equation are

$$\lambda = \begin{cases} 1 - \varepsilon \\ \frac{3}{2} + \frac{1}{2}\sqrt{1 + 4\varepsilon^2} \\ \frac{3}{2} - \frac{1}{2}\sqrt{1 + 4\varepsilon^2} \end{cases} \quad (5)$$

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

$$E_\varepsilon = \begin{cases} V_0(1 - \varepsilon) \\ V_0(2 + \varepsilon^2 + \mathcal{O}(\varepsilon^4)) \\ V_0(1 - \varepsilon^2 + \mathcal{O}(\varepsilon^4)) \end{cases} \quad (6)$$

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

$$V = V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \quad (7)$$

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

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

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

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

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

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

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

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

$$E_{3,2} = \frac{|\langle 20|V|30\rangle|^2}{V_0} = V_0 \varepsilon^2 \quad (12)$$

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

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

$$W_{11} = \langle 10|V|10\rangle = [1 \ 0 \ 0] V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = -\varepsilon V_0 \quad (13)$$

$$W_{21} = W_{12} = \langle 10|V|20\rangle = [1 \ 0 \ 0] V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0 \quad (14)$$

$$W_{22} = \langle 20|V|20\rangle = [0 \ 1 \ 0] V_0 \begin{bmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = 0 \quad (15)$$

$$W = \begin{bmatrix} -\varepsilon V_0 & 0 \\ 0 & 0 \end{bmatrix} \quad (16)$$

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