

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

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

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

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

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

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

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

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

The solutions of this equation are

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

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 $\sqrt{1+4\varepsilon^2} = 1 + 2\varepsilon^2 + \mathcal{O}(\varepsilon^4)$ so we get

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

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

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

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

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

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:

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

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

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

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

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

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

This correction term matches the ε^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 2×2 matrix, since the unperturbed state is only doubly degenerate. We get

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

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

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

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

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.