

## PERTURBATION OF 3-D SQUARE WELL

Link to: [physicspages home page](#).

To leave a comment or report an error, please use the auxiliary blog.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.8.

As a simple example of multiple degenerate perturbation theory, we start with the 3-d infinite square well and add a perturbation:

$$V = a^3 V_0 \delta\left(x - \frac{a}{4}\right) \delta\left(y - \frac{a}{2}\right) \delta\left(z - \frac{3a}{4}\right) \quad (1)$$

The wave functions of the unperturbed hamiltonian are

$$|0, n_x n_y n_z\rangle = \left(\frac{2}{a}\right)^{3/2} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \quad (2)$$

The ground state  $n_x = n_y = n_z = 1$  is non-degenerate, so we can use non-degenerate perturbation theory to find the change in energy. We get

$$E_{1,111} = \langle 0, 111 | V | 0, 111 \rangle \quad (3)$$

$$= \left(\frac{2}{a}\right)^3 V_0 a^3 \left[ \sin \frac{\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right]^2 \quad (4)$$

$$= 2V_0 \quad (5)$$

The first excited state is triply degenerate, since two of the  $n$ s are 1 and the other is 2. We need to calculate the matrix  $W_{ij} = \langle 0, i_x i_y i_z | V | 0, j_x j_y j_z \rangle$ . We take the elements in the order  $|0, 211\rangle$ ,  $|0, 121\rangle$  and  $|0, 112\rangle$ . We then get

$$W_{11} = \langle 0, 211 | V | 0, 211 \rangle \quad (6)$$

$$= \left(\frac{2}{a}\right)^3 V_0 a^3 \left[ \sin \frac{2\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right]^2 \quad (7)$$

$$= 4V_0 \quad (8)$$

$$W_{12} = \langle 0, 211 | V | 0, 121 \rangle \quad (9)$$

$$= \left(\frac{2}{a}\right)^3 V_0 a^3 \left[ \sin \frac{2\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right] \left[ \sin \frac{\pi}{4} \sin \frac{2\pi}{2} \sin \frac{3\pi}{4} \right] \quad (10)$$

$$= 0 \quad (11)$$

We can work out the other elements the same way and get

$$W = 4V_0 \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix} \quad (12)$$

The eigenvalues of the matrix  $W/4V_0$  are obtained from

$$(1 - \lambda)(-\lambda)(1 - \lambda) + \lambda = 0 \quad (13)$$

$$\lambda = 0, 0, 2 \quad (14)$$

Thus the triply degenerate unperturbed state splits into a non-degenerate state with first order energy correction of  $8V_0$  and a doubly degenerate state with the original energy.

The special states are found from the normalized eigenvectors of  $W$  which are

$$\frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (15)$$

So the states are

$$\frac{1}{\sqrt{2}} (-|0, 211\rangle + |0, 112\rangle) (E_1 = 8V_0) \quad (16)$$

$$\frac{1}{\sqrt{2}} (|0, 211\rangle + |0, 112\rangle) (E_1 = 0) \quad (17)$$

$$|0, 121\rangle (E_1 = 0) \quad (18)$$