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:

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

The wave functions of the unperturbed hamiltonian are

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

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

$$E_{1,111} = \langle 0,111|\, V\, |0,111\rangle \tag{3}$$

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

$$= 2V_0 \tag{5}$$

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

$$W_{11} = \langle 0,211|V|0,211\rangle \tag{6}$$

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

$$= 4V_0 \tag{8}$$

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

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

$$= 0 \tag{11}$$

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

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

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

$$(1-\lambda)(-\lambda)(1-\lambda)+\lambda = 0 \tag{13}$$

$$\lambda = 0,0,2 \tag{14}$$

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

$$\frac{1}{\sqrt{2}}\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{15}$$

So the states are

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

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

$$|0,121\rangle\,(E_1 = 0) \tag{18}$$