

PERTURBATION OF 3-D SQUARE WELL

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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:

$$(0.1) \quad V = a^3 V_0 \delta\left(x - \frac{a}{4}\right) \delta\left(y - \frac{a}{2}\right) \delta\left(z - \frac{3a}{4}\right)$$

The wave functions of the unperturbed hamiltonian are

$$(0.2) \quad |0, n_x n_y n_z\rangle = \left(\frac{2}{a}\right)^{3/2} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

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

$$(0.3) \quad E_{1,111} = \langle 0, 111 | V | 0, 111 \rangle$$

$$(0.4) \quad = \left(\frac{2}{a}\right)^3 V_0 a^3 \left[\sin \frac{\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right]^2$$

$$(0.5) \quad = 2V_0$$

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

$$(0.6) \quad W_{11} = \langle 0,211|V|0,211\rangle$$

$$(0.7) \quad = \left(\frac{2}{a}\right)^3 V_0 a^3 \left[\sin \frac{2\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right]^2$$

$$(0.8) \quad = 4V_0$$

$$(0.9) \quad W_{12} = \langle 0,211|V|0,121\rangle$$

$$(0.10) \quad = \left(\frac{2}{a}\right)^3 V_0 a^3 \left[\sin \frac{2\pi}{4} \sin \frac{\pi}{2} \sin \frac{3\pi}{4} \right] \left[\sin \frac{\pi}{4} \sin \frac{2\pi}{2} \sin \frac{3\pi}{4} \right]$$

$$(0.11) \quad = 0$$

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

$$(0.12) \quad W = 4V_0 \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

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

$$(0.13) \quad (1 - \lambda)(-\lambda)(1 - \lambda) + \lambda = 0$$

$$(0.14) \quad \lambda = 0, 0, 2$$

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

$$(0.15) \quad \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

So the states are

$$(0.16) \quad \frac{1}{\sqrt{2}} (-|0,211\rangle + |0,112\rangle) (E_1 = 8V_0)$$

$$(0.17) \quad \frac{1}{\sqrt{2}} (|0,211\rangle + |0,112\rangle) (E_1 = 0)$$

$$(0.18) \quad |0,121\rangle (E_1 = 0)$$