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:

$$V=a^{3}V_{0}\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{2}\right)\delta\left(z-\frac{3a}{4}\right) \tag{1}$$

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

$$\begin{aligned}
E_{1,111} &= \left\langle 0,111\right|V\left|0,111\right\rangle && (3)\\
&= \left(\frac{2}{a}\right)^{3}V_{0}a^{3}\left[\sin\frac{\pi}{4}\sin\frac{\pi}{2}\sin\frac{3\pi}{4}\right]^{2} && (4)\\
&= 2V_{0} && (5)
\end{aligned}$$

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 $\left|0,211\right\rangle$, $\left|0,121\right\rangle$ and $\left|0,112\right\rangle$. 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

$$\frac{1}{\sqrt{2}}(-|0,211\rangle + |0,112\rangle)\,(E_1 = 8V_0) \tag{16}$$
$$\frac{1}{\sqrt{2}}(|0,211\rangle + |0,112\rangle)\,(E_1 = 0) \tag{17}$$
$$|0,121\rangle\,(E_1 = 0) \tag{18}$$