PERTURBING THE 3-D HARMONIC OSCILLATOR

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.30.

Here's an example of perturbation theory applied to the 3-d harmonic oscillator. Using separation of variables, the stationary states in 3-d are just products of the 1-d states:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-m\omega x^2/2\hbar} \tag{1}$$

where H_n is the nth Hermite polynomial. The first two Hermite polynomials are

$$H_0(x) = 1 \tag{2}$$
$$H_1(x) = 2x \tag{3}$$

Thus the ground state in 3-d is (where the notation is $\psi_{n_x n_y n_z}$) :

$$\psi_{000} = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega x^2/2\hbar} e^{-m\omega y^2/2\hbar} e^{-m\omega z^2/2\hbar} \tag{4}$$

The first excited state is triply degenerate, since the excitation can be in any of the three coordinates. We get

$$\psi_{100} = \frac{2}{\pi^{3/4}} \left(\frac{m\omega}{\hbar}\right)^{5/4} x e^{-m\omega x^2/2\hbar} e^{-m\omega y^2/2\hbar} e^{-m\omega z^2/2\hbar} \tag{5}$$
$$\psi_{010} = \frac{2}{\pi^{3/4}} \left(\frac{m\omega}{\hbar}\right)^{5/4} y e^{-m\omega x^2/2\hbar} e^{-m\omega y^2/2\hbar} e^{-m\omega z^2/2\hbar} \tag{6}$$
$$\psi_{001} = \frac{2}{\pi^{3/4}} \left(\frac{m\omega}{\hbar}\right)^{5/4} z e^{-m\omega x^2/2\hbar} e^{-m\omega y^2/2\hbar} e^{-m\omega z^2/2\hbar} \tag{7}$$

Now suppose we introduce a perturbation given by

$$H' = \lambda x^2 yz \tag{8}$$

for some constant λ. We can use non-degenerate perturbation theory to calculate the correction to the energy in the ground state. This gives

$$E_{000,1} = \langle \psi_{000} | H' | \psi_{000} \rangle \tag{9}$$

$$= \lambda \int\int\int |\psi_{000}(x,y,z)|^2 x^2 yz dx dy dz \tag{10}$$

The integrals over y and z are zero, since ψ_{000} is an even function over all three coordinates and H' is odd in y and z. Thus

$$E_{000,1} = 0 \tag{11}$$

and there is no correction to the ground state energy to first order.

For the first excited state, we need to use the degenerate theory which means we need to calculate the matrix elements $W_{ab} = \langle n_x n_y n_z | H' | m_x m_y m_z \rangle$ for the 3 degenerate first excited states. These matrix elements are just the means of the coordinates or their squares, that is

$$W_{ab} = \lambda \langle n_x | x^2 | m_x \rangle \langle n_y | y | m_y \rangle \langle n_z | z | m_z \rangle \tag{12}$$

where the ns and ms must be chosen so that they make up one of the three degenerate states above. (That is, one each of the ns and ms must be 1 and the other two are 0.)

We've worked out some of these elements before, in particular in the 1-d case:

$$\langle n|x|n' \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n'+1}\,\delta_{n,n'+1} + \sqrt{n'}\,\delta_{n,n'-1} \right) \tag{13}$$

This shows that all the diagonal elements of W are zero, so we need look only at the off-diagonal elements. The quantity $\langle n_x | x^2 | m_x \rangle = 0$ if $n_x \neq m_x$ since the integrand contains a factor of x^3 which is an odd function. Thus the only non-zero elements must have $n_x = m_x$, $n_y \neq m_y$ and $n_z \neq m_z$. The only elements that satisfy these conditions are $W_{010,001} = \lambda \langle 0 | x^2 | 0 \rangle \langle 1 | y | 0 \rangle \langle 0 | z | 1 \rangle$ and $W_{001,010} = \lambda \langle 0 | x^2 | 0 \rangle \langle 0 | y | 1 \rangle \langle 1 | z | 0 \rangle$. For the last two factors we can use the formula above, while for $\langle 0 | x^2 | 0 \rangle$ we can use an earlier result:

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega} \tag{14}$$

$$\langle 0|y|1\rangle = \sqrt{\frac{\hbar}{2m\omega}} \tag{15}$$

$$\langle 1|z|0\rangle = \sqrt{\frac{\hbar}{2m\omega}} \tag{16}$$

Thus

$$W = \lambda \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \left(\frac{\hbar}{2m\omega}\right)^2 \\ 0 & \left(\frac{\hbar}{2m\omega}\right)^2 & 0 \end{bmatrix} \tag{17}$$

The energy corrections are the eigenvalues of W, which are

$$E_1 = 0, \pm\lambda \left(\frac{\hbar}{2m\omega}\right)^2 \tag{18}$$

Thus the perturbation splits the degeneracy, leaving one energy the same and moving the other two on either side of the original energy.