3. (Quantum Mechanics)

A particle in an infinite cubic well.

(a) Find the exact energies and wave functions of the ground and the first excited states and specify the degeneracies for the infinite cubic potential

$$V(x, y, z) = \begin{cases} 0 & 0 < x < L,\, 0 < y < L,\, 0 < z < L \\ \infty & \text{otherwise} \end{cases}$$

Now add the perturbation to the infinite cubic well:

$$H_p = V_0 L^3 \delta\left(x - \frac{L}{4}\right) \delta\left(y - \frac{3L}{4}\right) \delta\left(z - \frac{L}{4}\right)$$

(b) Using first order perturbation theory, calculate the energy of the ground state.

(c) Using first order *degenerate* perturbation theory, calculate the energy of the first excited state.

Solution: *Solution by Audrey Farrell*

(a) The 3D Schrödinger equation is separable into three independent 1D particle-in-a-box problems with well-known solutions:

$$\frac{d^2\psi}{dq_i^2} + k_i^2\psi = 0, \quad k_i^2 = \frac{2mE_i}{\hbar^2} \quad \rightarrow \quad \psi_{ni} = \sqrt{\frac{2}{L}}\sin\left(\frac{n_i\pi}{L}q_i\right), \quad \epsilon_{ni} = \frac{n_i^2\pi^2\hbar^2}{2mL^2}$$

Putting these together the total wavefunctions are

$$\psi_{n_xn_yn_z}(x,y,z) = \left(\frac{2}{L}\right)^{\frac{3}{2}}\sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}y\right)\sin\left(\frac{n_z\pi}{L}z\right)$$

with corresponding total energies

$$\epsilon_{n_xn_yn_z} = \epsilon_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \quad n^2 = n_x^2 + n_y^2 + n_z^2$$

The ground state is nondegenerate with $n_x = n_y = n_z = 1$, and corresponding energy $\epsilon_1 = \epsilon_{111} = \frac{3\pi^2\hbar^2}{2mL^2}$.

The first excited state is 3-fold degenerate with $\epsilon_{112} = \epsilon_{121} = \epsilon_{211} = \frac{6\pi^2\hbar^2}{2mL^2}$

(b) The first order correction to the ground state energy is given by $\Delta\epsilon_1^{(1)} = \langle\psi_1^{(0)}|H_p|\psi_1^{(0)}\rangle$, so

$$\begin{aligned}\langle H_p\rangle &= \int_0^L\int_0^L\int_0^L dx\,dy\,dz\,\psi_1^*(x,y,z)\,V_0L^3\,\delta\left(x-\frac{L}{4}\right)\delta\left(y-\frac{3L}{4}\right)\delta\left(z-\frac{L}{4}\right)\psi_1(x,y,z)\\ &= V_0L^3\left|\psi_1\left(\frac{L}{4},\frac{3L}{4},\frac{L}{4}\right)\right|^2 = 8V_0\sin^2\left(\frac{3\pi}{4}\right)\sin^2\left(\frac{3\pi}{4}\right)\sin^2\left(\frac{3\pi}{4}\right)\end{aligned}$$