HW #5 Answers

1. $\hat{L}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$

Because $\frac{\hbar}{i}\frac{\partial}{\partial z}$ and $\frac{\hbar}{i}\frac{\partial}{\partial z}$ are Hermitian, so is $\hat{L}_x$.

$\hat{x}\hat{p}_x = \frac{\hbar}{i}x\frac{\partial}{\partial x}$

This is not Hermitian as $(\hat{x}\hat{p}_x)^T = \hat{p}_x x$

2. Box with sloped bottom $V = ax$ for $0 \le x \le l$

$$\phi_1 = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi x}{l}\right), \quad \phi_2 = \sqrt{\frac{2}{l}}\sin\left(\frac{2\pi x}{l}\right)$$

The Hamiltonian matrix is $\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$

$$H_{11} = \langle\phi_1|H^0 + V|\phi_1\rangle = E_1^{(0)} + \langle\phi_1|V|\phi_1\rangle$$

$$H_{22} = \langle\phi_2|H^0 + V|\phi_2\rangle = E_2^{(0)} + \langle\phi_2|V|\phi_2\rangle$$

$$H_{12} = H_{21} = \langle\phi_1|H^0 + V|\phi_2\rangle = \langle\phi_1|V|\phi_2\rangle$$

$$\langle\phi_1|V|\phi_1\rangle = \frac{2a}{l}\frac{l^2}{4} = \frac{al}{2}$$

$$\langle\phi_2|V|\phi_2\rangle = \frac{2a}{l}\frac{l^2}{4} = \frac{al}{2}$$

$$\langle\phi_1|V|\phi_2\rangle = \frac{2a}{l}\left(-\frac{8l^2}{9\pi^2}\right) = -\frac{16al}{9\pi^2}$$

$$H_{11} = \frac{h^2}{8ml^2} + \frac{al}{2}, \quad H_{22} = \frac{4h^2}{8ml^2} + \frac{al}{2}$$

$$E_\pm = \frac{H_{11} + H_{22}}{2} \pm \frac{1}{2}\sqrt{(H_{11} - H_{22})^2 + 4H_{12}^2}$$

$$E_\pm = \frac{\frac{5h^2}{8ml^2} + al}{2} \pm \frac{1}{2}\sqrt{\left(\frac{3h^2}{8ml^2}\right)^2 + 4\left(\frac{16al}{9\pi^2}\right)^2}$$

If we assume that the perturbation is small compared to $|H_{11} - H_{22}|$, we can use PT to estimate the coefficients.

$$c_2 = \frac{H_{12}}{H_{11}-H_{22}}$$ for the correction to the ground state

$$c_2 = \frac{\frac{-16al}{9\pi^2}}{\frac{-3h^2}{8ml^2}} = \frac{16al}{9\pi^2}\frac{8ml^2}{3h^2} = \frac{16al}{9\pi^2}\frac{8ml^2}{3\hbar^2 4\pi^2}$$

$$= \frac{32\,mal^3}{27\pi^4\hbar^2} \rightarrow \frac{32}{27}\frac{al^3}{\pi^4} \text{ in a.u.}$$

Suppose $l = 10$ a.u., $a = .1$

$c_2 \rightarrow \frac{32}{27}\frac{100}{\pi^4}$. This is comparable to 1. Note $c_1 = 1$ in intermediate normalization. so for my choice of parameters, this is not a small perturbation.

With $l = 5$ a.u. or $a = .01$, it would be small.

3. $\psi_{2s} = \frac{1}{4\sqrt{2\pi}}(2-r)e^{-r/2}$, $\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} z e^{-r/2}$

$$\int \psi_{2s}\, z\, \psi_{2p_z} r^2 \sin\theta\, dr\, d\theta\, d\phi = \frac{1}{16(2\pi)}\int (2-r)(r\cos\theta)^2 r^2 e^{-r} \sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{2\pi}{16\, 2\pi}\int_0^\infty r^4(2-r)e^{-r}dr \int_0^\pi \cos^2\theta \sin\theta\, d\theta = \frac{2}{3}\frac{1}{16}\int_0^\infty r^4(2-r)e^{-r}dr$$

$$= \frac{1}{24}(-72) = -3$$

E (in atomic units) $= -\frac{1}{8} - 3\varepsilon$

The wavefunction is $\frac{1}{\sqrt{2}}(\psi_{2s} + \psi_{2p_z})$

Note that a typical electric field is 10^{-5} a.u.

$$\underline{H} = \begin{pmatrix} \langle 2s|H^\circ|2s\rangle & \langle 2s|V|2p_z\rangle \\ \langle 2s|V|2p_z\rangle & \langle 2p_z|H^\circ|2p_z\rangle \end{pmatrix}$$