1.) In class, we derived the Hydrogen wavefunction

$$|\psi_{n\ell}\rangle_{norm} = (-i)^{n-\ell-1}\left(\frac{na_0}{2}\right)^{n-1}\sqrt{\frac{(2n-1)!(n-\ell-1)!}{(n+\ell)!}}\,\frac{1}{\hat{r}^\ell}\,P_h^\ell(\hat{r}_x,\hat{r}_y,\hat{r}_z)\left(\frac{2\hat{r}}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2\hat{r}}{na_0}\right)|\phi_n\rangle.$$

a) We want to look at $|\psi_{21}\rangle = \frac{a_0}{\hat{r}}P_h^1(\hat{r}_x,\hat{r}_y,\hat{r}_z)\left(\frac{\hat{r}}{a_0}\right)^1 L_0^3\left(\frac{\hat{r}}{a_0}\right)|\phi_2\rangle$

recall $L_0^3 = 1$ and we pick $P_h^1(\hat{r}_x,\hat{r}_y,\hat{r}_z) = \sqrt{\frac{3}{4\pi}}\hat{r}_\alpha$ a p-wave state

so $|\psi_{21}\rangle_{norm} = \sqrt{\frac{3}{4\pi}}\hat{r}_\alpha|\phi_2\rangle \qquad \alpha = x, y, \text{ or } z$

Compute $\langle p_x, p_y, p_z|\psi_{21}\rangle_{norm} = \psi_{21}(p_x,p_y,p_z)$

Recall $\hat{p}_\alpha|\phi_2\rangle = \frac{i\hbar}{2a_0}\frac{\hat{r}_\alpha}{\hat{r}}|\phi_2\rangle$

Start by re writing $\langle\vec{p}|\hat{r}_x|\phi_2\rangle = \sqrt{\frac{3}{4\pi}}\frac{2a_0}{i\hbar}\langle\vec{p}|\hat{r}\,\hat{p}_\alpha|\phi_2\rangle$ using the above relation.

Use the commutator $[\hat{p}_\alpha,\hat{r}] = -i\hbar\frac{\hat{r}_\alpha}{\hat{r}}$ to show

$$\psi_{21}(\vec{p}) = \sqrt{\frac{3}{4\pi}}\frac{2a_0 p_\alpha}{i\hbar}\langle\vec{p}|\hat{r}|\phi_2\rangle + \sqrt{\frac{3}{4\pi}}2a_0\langle\vec{p}|\frac{\hat{r}_\alpha}{\hat{r}}|\phi_2\rangle$$

You need one more trick to get through — write $\hat{r} = \sum_\alpha \hat{r}_\alpha\frac{\hat{r}_\alpha}{\hat{r}}$ and replace $\frac{\hat{r}_\alpha}{\hat{r}}|\phi_2\rangle = \frac{i\hbar}{2a_0}\hat{p}_\alpha|\phi_2\rangle$ etc.

Note further that you should calculate $\langle\vec{p}|\hat{r}|\phi_2\rangle$ separately and substitute the result in to the final answer. You will end up at the end needing to compute $\langle\vec{p}|\phi_2\rangle$, which can be done similar to how we did this in lecture 11.

Finish the problem to compute $\psi_{21}(\vec{p})$ (You do not need to evaluate $\langle 0_p|\phi_2\rangle$)

b) $|\psi_{20}\rangle = -i\,a_0\frac{\sqrt{3}}{\sqrt{4\pi}}L_1^1\left(\frac{\hat{r}}{a_0}\right)|\phi_2\rangle \qquad L_1^1\left(\frac{\hat{r}}{a_0}\right) = 2-\frac{\hat{r}}{a_0} \qquad P_h^0(\hat{r}_x,\hat{r}_y,\hat{r}_z) = \frac{1}{\sqrt{4\pi}}$

so $\psi_{20}(\vec{p}) = -i\frac{\sqrt{3}}{\sqrt{4\pi}}a_0\langle\vec{p}|2-\frac{\hat{r}}{a_0}|\phi_2\rangle$

Use techniques similar to what we did above to find $\psi_{20}(\vec{p})$.

2.) Using $\hat{H} = \hat{H}_0 + \hat{V}$ $\quad V_{nm} = \langle n|\hat{V}|m\rangle$

we have the non degenerate PT through 4th order is

$$E_n = E_n^0 + V_{nn} + \underbrace{\sum_{m\neq n} \frac{|V_{nm}|^2}{E_n^0 - E_m^0}}_{\text{second}} + \sum_{m\neq n}\sum_{m'\neq n} \frac{V_{nm}V_{mm'}V_{m'n}}{(E_n^0-E_m^0)(E_n^0-E_{m'}^0)} - V_{nn}\sum_{m\neq n}\frac{|V_{nm}|^2}{(E_n^0-E_m^0)^2}$$

(first; second; third)

Fourth:

$$+ \sum_{m\neq n}\sum_{m'\neq n}\sum_{m''\neq n} \frac{V_{nm}V_{mm'}V_{m'm''}V_{m''n}}{(E_n^0-E_m^0)(E_n^0-E_{m'}^0)(E_n^0-E_{m''}^0)}$$

$$- \sum_{m\neq n}\sum_{m'\neq n} \frac{|V_{nm}|^2|V_{nm'}|^2}{(E_n^0-E_m^0)^2(E_n^0-E_{m'}^0)}$$

$$- V_{nn}\sum_{m\neq n}\sum_{m'\neq n} \frac{V_{nm}V_{mm'}V_{m'n}}{(E_n^0-E_m^0)(E_n^0-E_{m'}^0)}\left[\frac{1}{E_n^0-E_m^0} + \frac{1}{E_n^0-E_{m'}^0}\right]$$

$$+ V_{nn}^2 \sum_{m\neq n}\frac{|V_{nm}|^2}{(E_n^0-E_m^0)^3}$$

Take $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 \qquad \hat{V} = \frac{1}{2}\Delta k\,\hat{x}^2$

a.) Compute E_n exactly, and Taylor series expand in a series in Δk through fourth order in Δk.

b.) Compute E_n through fourth order in $\hat{V}$ using the above formulas for RS PT.

c.) Compute E_n to second order in Wigner-Brillouin perturbation theory for the ground state only ($n=0$).

d.) Plot E (2nd order RS), E (4th order RS), E (2nd order, WB), Taylor series through 4th order and the exact result for $0 \le \frac{\Delta k}{k} \le 3$. (For the ground state only, $n=0$).

Comment on the quality of the different approximations.

3.) Consider the isotropic simple harmonic oscillator $\hat{H} = \frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m} + \frac{1}{2}k(\hat{x}^2+\hat{y}^2+\hat{z}^2)$ (3)

a.) Using the factorization method in cartesian coordinates, find the energy eigenvalues.

b.) Rewrite $\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2m\hat{r}^2} + \frac{1}{2}k\hat{r}^2$

and find the eigenvalues using factorization in spherical coordinates. Recall $\hat{H}_\ell = \frac{\hat{p}_r^2}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2m\hat{r}^2} + \frac{1}{2}k\hat{r}^2$

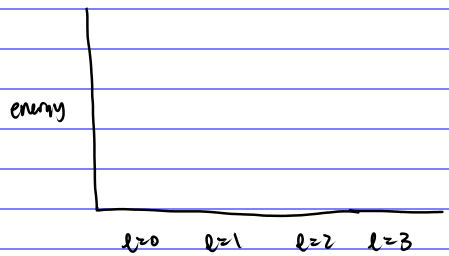
Verify they are the same as those found in a.)

Hint: use $\hat{B}_r^\dagger(\ell) = \frac{1}{\sqrt{2m}}\left(\hat{p}_r + i\left[m\omega\alpha\hat{r} + \frac{\hbar\beta}{\hat{r}}\right]\right)$

with both α and β nonzero. Do not compute wfs.

Note: for each ℓ, compute $H_n^{\ell,\text{eff}}$ to find the energy from the constant term.

c.) Plot the energy levels from b as



4.) Perturbed spherical harmonic oscillator

a.) Find the ground-state wave function (use either cartesian or spherical coordinates)

b) add a perturbation $\hat{V} = \frac{1}{2}\delta k\hat{x}^2$

The ground state is non degenerate.

Compute E_{gs} through second order in Rayleigh-Schrödinger PT.

c.) Compute the exact energy in the cartesian basis and compare to the perturbative energy.