PHYS 5002: Homework 6

1 Momentum space hydrogen wavefunctions

In class, we derived an identity for the hydrogen energy eigenfunction in a form reminiscent of the position wavefunction:

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

a.) We want to look at

$$|\psi_{21}\rangle = \frac{a_0}{\hat{r}}P_n^1(\hat{r}_x,\hat{r}_y,\hat{r}_z)\left(\frac{\hat{r}}{a_0}\right)L_0^3\left(\frac{\hat{r}}{a_0}\right)|\phi_2\rangle$$

Recall $L_0^3 = 1$ and choose $P_n^1(\hat{r}_x,\hat{r}_y,\hat{r}_z) = \sqrt{\frac{3}{4\pi}}\hat{r}_\alpha$ which is a p-wave state. So,

$$|\psi_{21}\rangle_{norm} = \sqrt{\frac{3}{4\pi}}\hat{r}_\alpha|\phi_2\rangle$$

for $\alpha = x, y,$ or z.

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

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

Use this to rewrite $\langle\mathbf{p}|\hat{r}_x|\phi_2\rangle = \sqrt{\frac{3}{4\pi}}\frac{2a_0}{i\hbar}\langle\mathbf{p}|\hat{r}\hat{p}_\alpha|\phi_2\rangle$.

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

$$\psi_{21}(\mathbf{p}) = \sqrt{\frac{3}{4\pi}}\frac{2a_0p_\alpha}{i\hbar}\langle\mathbf{p}|\hat{r}|\phi_2\rangle + \sqrt{\frac{3}{4\pi}}2a_0\left\langle\mathbf{p}\middle|\frac{\hat{r}_\alpha}{\hat{r}}\middle|\phi_2\right\rangle$$

Now, one last trick is needed: Write $\hat{r} = \sum_\alpha\frac{\hat{r}_\alpha\hat{r}_\alpha}{\hat{r}}$ 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 $\langle\mathbf{p}|\hat{r}|\phi_2\rangle$ separately and substitute the result into the final answer. You will end up needing to compute $\langle\mathbf{p}|\phi_2\rangle$, which can be done similar to how we did this in **Lecture 11**. Finish the problem to compute $\psi_{21}(\mathbf{p})$. You do not need to evaluate $\langle 0_p|\phi_2\rangle$.

b.) Now consider $|\psi_{20}\rangle = -ia_0\sqrt{\frac{3}{4\pi}}L_1^1\left(\frac{\hat{r}}{a_0}\right)|\phi_2\rangle$ where $L_1^1\left(\frac{\hat{r}}{a_0}\right) = 2 - \frac{\hat{r}}{a_0}$ so

$$\psi_{20}(\mathbf{p}) = -i\sqrt{\frac{3}{4\pi}}a_0\left\langle\mathbf{p}\middle|\left(2-\frac{\hat{r}}{a_0}\right)\middle|\phi_2\right\rangle.$$

Calculate $\psi_{20}(\mathbf{p})$ using the same techniques as above.

2 Comparing different perturbation theories

Using $\hat{H} = \hat{H}_0 + \hat{V}$ where $V_{nm} = \left\langle n \middle| \hat{V} \middle| m \right\rangle$ we have the non-degenerate perturbation theory through fourth order is

$E_n = E_n^0 +$ first order correction + second order correction + third order correction + fourth order correction

where

$$\text{first order correction} = V_{nn}$$

$$\text{second order correction} = \sum_{m \neq n} \frac{V_{mn}}{E_n^0 - E_m^0}$$

$$\text{third order correction} = \sum_{m \neq n} \sum_{m \neq n'} \frac{V_{nm} V_{mm'} V_{m'n}}{(E_n^0 - E_m^0)(E_n^0 - E_{m'}^0)} - V_{nn} \sum_{m \neq n} \frac{|V_{nm}|^2}{(E_n^0 - E_m^0)^2}$$

and last but not least,

$$\text{fourth order correction} = \sum_{m = \neq n} \sum_{m' \neq n} \sum_{m'' \neq n} \frac{V_{nm} V_{mm'} V_{m'm''} V_{m''n}}{(E_n^0 - E_m^0)(E_n^0 - E_{m'}^0)(E_n^0 - E_{m''}^0)} - \sum_{m \neq n} \sum_{m' = n} \frac{|V_{nm}|^2 |V_{nm'}|^2}{(E_n^0 - E_m^0)(E_n^0 - E_{m'}^0)}$$
$$- V_{nn} \sum_{m \neq n} \sum_{m' \neq n} \frac{V_{nm} V_{mm'} V_{m'n}}{(E_n^0 - E_m^0)(E_n^0 - E_{m'}^0)} \left(\frac{1}{E_n^0 - E_m^0} + \frac{1}{E_n^0 - E_{m'}^0} \right) + V_{nn}^2 \sum_{m \neq n} \frac{|V_{nm}|^2}{(E_n^0 - E_m^0)^3}$$

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

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

b.) Compute E_n through fourth order in $\hat{V}$ using the above formula for Rayleigh-Schrödinger perturbation theory.

c.) Compute E_n to second in Wigner-Brillouin perturbation theory for the <u>ground state only</u>.

d.) Plot E(second order RS), E(fourth order RS), E(second order WB), and the Taylor series through fourth order for $0 \leq \frac{\Delta k}{k} \leq 3$ (for the ground state only). Comment on the quality of the different approximations.

3 Isotropic harmonic oscillator

Consider the isotropic simple harmonic oscillator:

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \frac{1}{2} k (\hat{x}^2 + \hat{y}^2 + \hat{z}^2)$$

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 the factorization method in spherical coordinates. Recall

$$\hat{H}_l = \frac{\hat{p}_r^2}{2m} + \frac{\hbar^2 l(l+1)}{2m\hat{r}^2} + \frac{1}{2} k \hat{r}^2$$

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

<u>HINT:</u> Use

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

with both α and β both nonzero.

c.) Plot the energy levels for discrete values of l.

4 Perturbed spherical harmonic oscillator

a.) Find the ground state wavefunction (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 perturbation theory.

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