P7502 HW3

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Problem 1

1. We have the equation

$$E_n^1 = \langle n^0 | H^1 | n^0 \rangle \tag{1}$$

where n^0 is just the nth state of the unperturbed oscillator. Note that

$$\begin{aligned}
E_n^1 &= \langle n^0 | \lambda x^4 | n^0 \rangle \\
&= \lambda \langle n^0 | (\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a))^4 | n^0 \rangle \\
&= \lambda \left(\frac{\hbar}{2m\omega}\right)^2 \langle n^0 | (a^2 {a^\dagger}^2 + a^\dagger a^2 a^\dagger + a a^\dagger a a^\dagger + a^\dagger a a^\dagger a + a {a^\dagger}^2 a + {a^\dagger}^2 a^2) | n^0 \rangle \\
&\text{By exploiting commutating relation} [a, a^\dagger] = 1 \\
&= \lambda \left(\frac{\hbar}{2m\omega}\right)^2 (6(n+1)(n+2) - 12(n+1) + 3) \\
&= \frac{3\lambda\hbar^2}{4m^2\omega^2}(2n^2 + 2n + 1) \checkmark
\end{aligned}$$

2. Because the first perterbation term E_n^1 scales with n^2, $\forall \lambda \in \mathbb{C}, \exists \lambda$ such that $E_n^1 > \Delta E_n$.

Physically, because our Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega x^2 + \lambda x^4$ will approach $H' = \frac{p^2}{2m} + \lambda x^4$ for n sufficiently large regardless how small a fixed λ. This means our potential term will be dominiated by the perterbation.

Problem 2

We have that $H = H^0 + H^1 = -\gamma S_z B_0 - \gamma S_x B$

Because the main magnetic field B_0 is in $\hat{z}$ direction, we recogonize that the spin up state is going to be the ground state as it has the lowest energy.

Therefore,

$$\begin{aligned}
E^1_+ &= \langle + | \, H^1 \, | + \rangle \\
&\doteq \frac{-\hbar\gamma B}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0
\end{aligned}$$

$$\begin{aligned}
E^2_+ &= \frac{\left| \langle + | \, H^1 \, | - \rangle \right|^2}{E^0_+ - E^0_-} \\
&= \frac{\gamma^2 B^2 \hbar^2}{4} \frac{1}{-\gamma B_0 \hbar} = -\frac{B^2 \hbar \gamma}{4 B_0}
\end{aligned}$$

$$\begin{aligned}
|+^1\rangle &= |+^0\rangle + \frac{\langle - | \, H_1 \, | + \rangle}{E^0_+ - E^0_-} \\
&= |+\rangle + \frac{B}{2B_0} \, |-\rangle
\end{aligned}$$

To compare the expanded exact solution, we first note that to get the exact answer, we just need to diagonalize
$H \doteq -\gamma \frac{\hbar}{2} \begin{pmatrix} B_0 & B \\ B & -B_0 \end{pmatrix}$ Because we only care about the ground state, we only select negative eigenvalue and its eigenvector. This gives $E = \frac{-\sqrt{B^2 + B_0^2}\hbar\gamma}{2}$ and $|n\rangle = |+\rangle - \frac{B}{-B_0 - \sqrt{B^2 + B_0^2}} \, |-\rangle$ We can expand our E

$$\begin{aligned}
E &= \frac{-\sqrt{B^2 + B_0^2}\hbar\gamma}{2} \\
&= -\frac{\hbar\gamma}{2} B_0 \sqrt{1 + \frac{B^2}{B_0^2}} \\
&\approx -\frac{\hbar\gamma}{2} (B_0 + \frac{B^2}{2B_0})
\end{aligned}$$

This agrees with our perterbation parameters where $E^0 = -\frac{\hbar\gamma B_0}{2}$, $E^1 = 0$, and $E^2 = -\frac{B^2 \hbar\gamma}{4B_0}$ We can expand our $|n\rangle$

$$\begin{aligned}
|n\rangle &= |+\rangle - \frac{B}{-B_0 - \sqrt{B^2 + B_0^2}} \, |-\rangle \\
&\approx |+\rangle + \frac{B}{2B_0 + \frac{B^2}{B_0}} \, |-\rangle \\
&\approx |+\rangle + \frac{B}{2B_0} \, |-\rangle
\end{aligned}$$

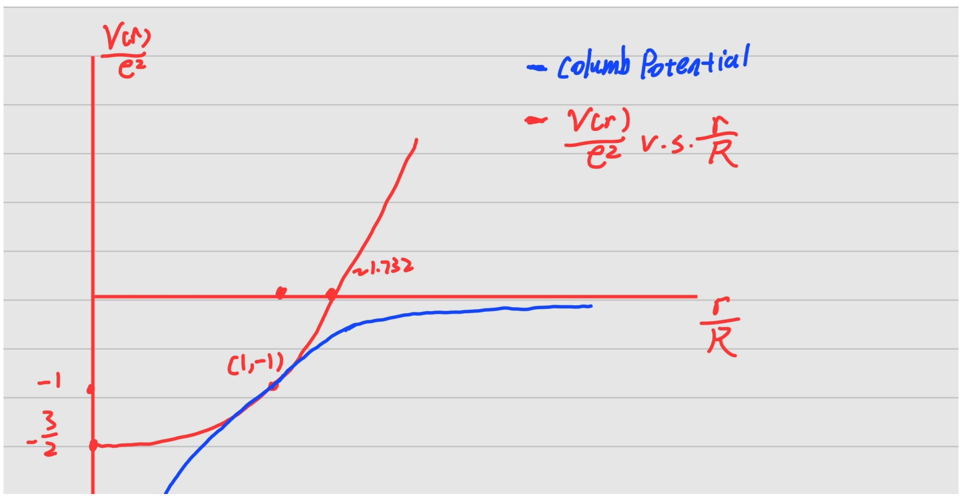
Which is exactly the same as $|+^1\rangle$ the first perterbed eigenstate.

Problem 3

for $r > R$, the problem returns to be Columb potential problem. Thus we conly consider the case where $r < R$ that corresponds to $V(r) = \frac{3e^2}{2R} + \frac{e^2r^2}{2R^3}$

We have $H^1 = V(r) - V_{\text{Columb}}(r) = -\frac{3e^2}{2R} + \frac{e^2r^2}{2R^3} + \frac{e^2}{r}$

$$\begin{aligned} E_1^1 &= \langle 100| H_1 |100\rangle \\ &= \int_0^{2\pi}\int_0^{\pi}\int_0^{R} e^{-2r/\alpha_0}\frac{1}{\pi a_0^3}(-\frac{3e^2}{2R} + \frac{e^2r^2}{2R^3} + \frac{e^2}{r})r^2\sin\theta \mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \\ &= \frac{4}{a_0^3}\left(\frac{1}{2}e^2R^2 - \frac{1}{2}e^2R^2 + \frac{1}{10}e^2R^2\right) \\ &= \frac{2e^2R^2}{5a_0^3} \end{aligned}$$



Notice that in our graphics of $V(r)$, the Columb potential is only similiar to our potential near $r = R$. I think this is fine, because for $r > R$, we define our potential to be the columb potential, and for $r << R$, the angular effective potential will likely dominate anyway.

Now for Numerical Estimation, we bring back the missing $\frac{1}{4\pi\epsilon_0}$

$$\begin{aligned} E_1^1 &\approx \frac{2}{5}e^2(1E-9\mu\text{m})^2/(5.3E-5\mu\text{m})^3\frac{1\text{eV}}{4\pi\cdot 55e^2\mu\text{m}} \\ &= 4\cdot 10^{-9}\text{eV} \end{aligned}$$

To figure out what change in mass would result in change in perterbation result, we first realize that the radius a_0 must change when we increase the mass of the particle. Using classical mech and Bhor's QUantization condtiion

$$\frac{e^2}{4\pi\epsilon_0 r^2} = m_\mu \frac{v^2}{r}$$
$$\Rightarrow r = \frac{4\pi\epsilon_0\hbar^2}{m_\mu e^2} = \frac{1}{200}a_0$$

Once we realized that our new radius is $\frac{1}{200}a_0$, we realize that our new perterbation term must be $200^3 = 8000000$ times stronger. Using previous result, this will grant us 0.032eV.

Note that Technically speaking, our eigenenergy E_n should also increase by a factor of 200. This still makes our perterbation term $200^2 = 40000$ times larger with respect to E^0.

Problem 4

1) We have

$$W = \frac{e^2}{R^3}[\mathbf{r_A}\cdot\mathbf{r_B} - 3(\mathbf{r_A}\cdot\hat{\mathbf{n}})(\mathbf{r_B}\cdot\hat{\mathbf{n}})] \tag{2}$$

A small parameter that would fit the problem would be $\lambda = \frac{a_0^3}{R^3} \propto \frac{W}{H^0}$. Because we hvae $R >>> \{r_a, r_B\} \propto a_0$. we must have that $\frac{a_0}{R^3}^3$ is a small parameter that compares W with H^0.

2) WLOG, we can choose $\hat{n}$ to be $\hat{z}$. This gives a specific equation representaion for W in Cartecian Coordinates

$$\begin{aligned}
W &= \frac{e^2}{R^3}[\mathbf{r_A}\cdot\mathbf{r_B} - 3(\mathbf{r_A}\cdot\hat{\mathbf{n}})(\mathbf{r_B}\cdot\hat{\mathbf{n}})] \\
&= \frac{e^2}{R^3}[x_A x_B + y_a y_B + z_A z_B - 3z_A z_B] \\
&= \frac{e^2}{R^3}[x_A x_B + y_a y_B - 2z_A z_B]
\end{aligned}$$

3) We can use the fact that our $|100_A;100_B\rangle$ is spehrically symmetric. and realize $W = H^1$ has two positive contribution in X, Y and 2 times negative contribution in Z. The spherical symmetric nature of the wave function means the contribution from all directions are the same. Therefore, the contribution of $X + Y - 2Z$ should be 0.

Alternatively, we just realize for each wavefuncion,

$$\int_0^{2\pi}\int_0^{\pi} \mathrm{d}\theta\mathrm{d}\phi \cos\phi\sin\theta + \sin\phi\sin\theta - 2\cos\theta = 0 \tag{3}$$

This makes physically sense because the first degree multiple expansion is between $E-$field and charges. However, the net charge of each Hydrogen atom is neutral.

4)

For our second order energy perterbation term E^2, we have the following equation

$$E_n^2 = \sum_m \frac{|\langle n^0| H^1 |m^0\rangle|^2}{E_n^0 - E_m^0} \tag{4}$$

First, we realize that our denominator is negative since $E_n^0 < E_m^0 \forall n \neq m$ as we set n to be the ground state.

Second, we realizee that our neumerator will at least have the factor $|\frac{e^2}{R^3}|^2$. Combing these two facts, we can say that $E_n^2 \propto -\frac{c}{R^6}$ for some $c > 0$.

5) As we have two pariticles in H,

$$\begin{aligned}
E_n^2 &= \sum_m \frac{|\langle n^0| H^1 |m^0\rangle|^2}{2E_n^0 - 2E_m^0} \\
E_n^2 &\approx \sum_m \frac{|\langle n^0| H^1 |m^0\rangle|^2}{2E_1} \text{by using identity} \\
&\approx \frac{|\langle n^0| H^1 H^1 |n^0\rangle|}{2E_1} \\
&\approx -\frac{e^4}{2E_1 R^6} \langle 100; 100| (X_A X_B + Y_A Y_B - 2Z_A Z_B)^2 |100; 100\rangle \\
\Rightarrow c &\propto \frac{e^2}{2|E_1|} \langle 100; 100| (X_A X_B + Y_A Y_B - 2Z_A Z_B)^2 |100; 100\rangle
\end{aligned}$$

6) Explicitly, we can integrate $X_A Y_A$explicitlly. Note that our radial part of the integration does not involve θ, ϕ, we can simply integrate our wavefunction over θ, ϕ

$$\begin{aligned}
&\int_0^\pi \int_0^{2\pi} \mathrm{d}\phi \mathrm{d}\theta {Y_0^0}^2 \sin\theta \sin\theta \sin\phi \sin\theta \cos\phi \\
&= \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \mathrm{d}\phi \mathrm{d}\theta \sin^3\theta \sin\phi \cos\phi \\
&= \frac{1}{4\pi} \int_0^{2\pi} \mathrm{d}\phi \sin\phi \cos\phi \cdot \int_0^\pi \mathrm{d}\theta \sin^3\theta
\end{aligned}$$

Where the $\mathrm{d}\phi$ integral is 0.

7) We have exlicitly

$$
\begin{aligned}
&\langle 100;100|\, R^2\, |100;100\rangle \\
&= \frac{1}{\pi a_0^3}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^4 \sin\theta \mathrm{d}\phi\mathrm{d}\theta\mathrm{d}r \\
&= 3a_0^2 \\
&\langle 100;100|\, Z^2\, |100;100\rangle \\
&= \frac{1}{\pi a_0^3}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^4 \sin\theta\cos^2\theta \mathrm{d}\phi\mathrm{d}\theta\mathrm{d}r \\
&= a_0^2 \\
&\langle 100;100|\, X^2\, |100;100\rangle \\
&= \frac{1}{\pi a_0^3}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^4 \sin\theta\sin^2\theta\cos^2\phi \mathrm{d}\phi\mathrm{d}\theta\mathrm{d}r \\
&= a_0^2 \\
&\langle 100;100|\, Y^2\, |100;100\rangle \\
&= \frac{1}{\pi a_0^3}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^4 \sin\theta\sin^2\theta\sin^2\phi \mathrm{d}\phi\mathrm{d}\theta\mathrm{d}r \\
&= a_0^2
\end{aligned}
$$

Note that the expetation value of each direction squared is just $\frac{1}{3}\langle R^2\rangle$

8) In Gaussian unit, energy $\propto e^2/r$. Therefore, for our unit to be in the unit of energy, we must have $p = 2$. As we have R^6 in the denominator and we want r^-1, we must have $q - 6 = -1 \to q = 5$