

1.) a) Consider that the Hamiltonian and the time reversal operator commutes

$$[H, \hat{\theta}] = 0$$

then for every energy eigenstates $|n\rangle$, the time reversed state $\hat{\theta}|n\rangle$ share the same energy.
Let $H|n\rangle = E_n|n\rangle$, and from the commutation operation

$$H\hat{\theta}|n\rangle - \hat{\theta}H|n\rangle = 0$$

$$H\hat{\theta}|n\rangle = \hat{\theta}H|n\rangle$$

Let $H|n\rangle = E_n|n\rangle$, and from the commutation relation

$$E\hat{\theta}|n\rangle = \hat{\theta}E|n\rangle$$

Therefore $|n\rangle$ and $\hat{\theta}|n\rangle$ share the same energy. If $|n\rangle$ represents the same state as $\hat{\theta}|n\rangle$, therefore they differ by a phase factor

$$\hat{\theta}|n\rangle = e^{i\delta}|n\rangle$$

Applying $\hat{\theta}$

$$\hat{\theta}^2|n\rangle = \hat{\theta}e^{i\delta}|n\rangle$$

$$= e^{-i\delta}\hat{\theta}|n\rangle$$

$$= e^{-i\delta}e^{i\delta}|n\rangle$$

$$= |n\rangle$$

this can never happen for any half integer j since

$$\hat{\theta}^2|j\text{-half integer}\rangle = -|j\text{-half integer}\rangle$$

therefore $|n\rangle$ and $\hat{\theta}|n\rangle$ must correspond to different states with the same energy. Therefore there is a 2 fold degeneracy.

b.) In an external magnetic field the Hamiltonian would have terms such as

$$S \cdot B, p \cdot A + A \cdot p; \quad B = \nabla \times A$$

the spin operator and momentum operator, S and p , are odd under time reversal. With the commutation relation would not be 0.

$$H\hat{\theta} \neq \hat{\theta}H$$

However for an external electric field we can set the vector potential to 0 so that the Hamiltonian wouldn't be affected so Kramers' degeneracy holds.

2.) We have the perturbation given by

$$V = \frac{e^2}{r} + \frac{e^2}{|\vec{r} + \vec{r}_2 - \vec{r}_1|} - \frac{e^2}{|\vec{r} + \vec{r}_2|} - \frac{e^2}{|\vec{r} - \vec{r}_1|}$$

expanding the denominators

$$V = \frac{e^2}{r} + \frac{e^2}{(\vec{r} \cdot \vec{r} + 2\vec{r} \cdot \vec{r}_2 + \vec{r}_2 \cdot \vec{r}_2)^{1/2}} - \frac{e^2}{(\vec{r} \cdot \vec{r} + 2\vec{r} \cdot \vec{r}_2 + \vec{r}_2 \cdot \vec{r}_2)^{1/2}} - \frac{e^2}{(\vec{r} \cdot \vec{r} + 2\vec{r} \cdot \vec{r}_1 + \vec{r}_1 \cdot \vec{r}_1)^{1/2}}$$

$$V = \frac{e^2}{r} + \frac{e^2}{\sqrt{r^2 + 2\vec{r} \cdot \vec{r}_2 + r_2^2}} - \frac{e^2}{\sqrt{r^2 + 2\vec{r} \cdot \vec{r}_2 + r_2^2}} - \frac{e^2}{\sqrt{r^2 + 2\vec{r} \cdot \vec{r}_1 + r_1^2}}$$

$$V = \frac{e^2}{r} \left[1 + \frac{1}{\sqrt{1 + \frac{2\vec{r}_2 \cdot \vec{r}_1}{r} + \frac{(\vec{r}_2 - \vec{r}_1)^2}{r^2}}} - \frac{1}{\sqrt{1 + \frac{2\vec{r}_2 \cdot \vec{r}_1}{r} + \frac{r_2^2}{r^2}}} - \frac{1}{\sqrt{1 - \frac{2\vec{r}_1 \cdot \vec{r}_1}{r} + \frac{r_1^2}{r^2}}} \right]$$

using the Taylor expansion

$$\frac{1}{\sqrt{1+\epsilon}} = 1 - \frac{\epsilon}{2} + \frac{3}{8}\epsilon^2 + O(\epsilon^3) \dots$$

the perturbation would expand as

$$V = \frac{e^2}{r} \left[1 + \left(1 - \frac{2\vec{r}_2 \cdot \vec{r}_1}{r} - \frac{(\vec{r}_2 - \vec{r}_1)^2}{2r^2} + \frac{3}{8} \left(\frac{2\vec{r}_2 \cdot \vec{r}_1}{r} + \frac{(\vec{r}_2 - \vec{r}_1)^2}{r^2} \right)^2 \right) - \left(1 - \frac{2\vec{r}_2 \cdot \vec{r}_1}{r} - \frac{r_2^2}{2r^2} + \frac{3}{8} \left(\frac{2\vec{r}_2 \cdot \vec{r}_1}{r} + \frac{r_2^2}{r^2} \right)^2 \right) - \left(1 + \frac{2\vec{r}_1 \cdot \vec{r}_1}{r} - \frac{r_1^2}{2r^2} + \frac{3}{8} \left(-\frac{2\vec{r}_1 \cdot \vec{r}_1}{r} + \frac{r_1^2}{r^2} \right)^2 \right) \right]$$

we would only keep terms that don't exceed $1/r^3$ in its overall contribution

$$V = \frac{e^2}{r} \left[1 + 1 - \frac{(\vec{r}_2 - \vec{r}_1)^2}{2r^2} + \frac{3}{2} \frac{(\vec{r}_2 - \vec{r}_1)^2}{r^2} - 1 + \frac{2\vec{r}_2 \cdot \vec{r}_1}{r} + \frac{r_2^2}{2r^2} - \frac{3}{2} \frac{r_2^2}{r^2} - 1 - \frac{2\vec{r}_1 \cdot \vec{r}_1}{r} + \frac{r_1^2}{2r^2} - \frac{3}{2} \frac{r_1^2}{r^2} \right]$$

$$V = \frac{e^2}{r} \left[\left(\frac{-\vec{r}_2 + \vec{r}_1 + \vec{r}_2 - \vec{r}_1}{r} \right) + \left(\frac{-r_2^2 + 2\vec{r}_2 \cdot \vec{r}_1 - r_1^2 + 3r_2^2 - 6\vec{r}_1 \cdot \vec{r}_2 + 3r_1^2 + r_2^2 - 3r_2^2 + r_1^2 - 3r_1^2}{2r^2} \right) \right]$$

$$V = \frac{e^2}{r} \left(\frac{2\vec{r}_1 \cdot \vec{r}_2 - 6\vec{r}_1 \cdot \vec{r}_2}{2r^2} \right) = \frac{e^2}{r^3} (x_1 x_2 + y_1 y_2 + z_1 z_2 - 3z_1 z_2)$$

$$V = \frac{e^2}{r^3} (x_1 x_2 + y_1 y_2 - 2z_1 z_2)$$

the first order perturbation is 0 while the 2nd order perturbation is non-vanishing

$$E_0^{(2)} = \sum_{k \neq 0} \frac{|\langle k^{(0)} | V | 0^{(0)} \rangle|^2}{E_0 - E_k}$$

this simplifies into

$$E_0^{(2)} = \frac{e^4}{r^6} \sum_{k \neq 0} \frac{|\langle k^{(0)} | x_1 x_2 + y_1 y_2 - 2z_1 z_2 | 0^{(0)} \rangle|^2}{E_0 - E_k}$$

Therefore there is a r^{-6} attractive potential between 2 atoms in their ground state.

3.) a) consider the Hamiltonian of SHO

$$H_0 = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 x^2$$

with perturbation

$$H' = f x$$

the Hamiltonian would then be

$$H = H_0 + H'$$

$$H = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 x^2 + f x$$

the first order perturbation theory

$$E_n^{(1)} = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

$$E_n^{(1)} = f \langle \psi_n^0 | x | \psi_n^0 \rangle$$

$$\boxed{E_n^{(1)} = 0}$$

the second order

perturbation theory is

$$E_n^{(2)} = \sum_{n' \neq n} \frac{|\langle \psi_{n'}^0 | f x | \psi_n^0 \rangle|^2}{E_n - E_{n'}}$$

$$= \sum_{n' \neq n} \frac{f^2 |\langle \psi_{n'}^0 | x | \psi_n^0 \rangle|^2}{E_n - E_{n'}}$$

$$= f^2 \frac{\hbar}{2m\omega} \sum_{n' \neq n} \frac{(\sqrt{n} \langle n' | n-1 \rangle + \sqrt{n+1} \langle n' | n+1 \rangle)^2}{E_n - E_{n'}}$$

the only non zero contribution is from $n' = n+1$, $n' = n-1$. Therefore,

$$E_n^{(2)} = f^2 \frac{\hbar}{2m\omega} \left(-\frac{n+1}{\hbar\omega} + \frac{n}{\hbar\omega} \right) = f^2 \left(\frac{\hbar}{2m\omega} \right) \left(\frac{1}{\hbar\omega} \right)$$

$$\boxed{E_0^{(2)} = \frac{f^2}{2m\omega^2}}$$

b) We have the Hamiltonian

$$H = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 x^2 + f x$$

we can rewrite this as

$$H = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 \left(x^2 + \frac{2f}{m\omega^2} x \right)$$

completing the square inside the parenthesis

$$H = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 \left(\left(x + \frac{f}{m\omega^2} \right)^2 - \left(\frac{f}{m\omega^2} \right)^2 \right)$$

letting $x \rightarrow x + \frac{f}{m\omega^2}$, we have

$$H = \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 \left(x^2 - \left(\frac{f}{m\omega^2} \right)^2 \right)$$

3) b.) We have the relation

$$\langle \psi | H | \psi \rangle = \langle \psi | E_n | \psi \rangle$$

therefore,

$$\langle \psi | \frac{1}{2} \frac{p^2}{m} + \frac{1}{2} m \omega^2 x^2 - \frac{1}{2} m \omega^2 \left(\frac{f}{m \omega^2} \right)^2 | \psi \rangle = \langle \psi | E_n | \psi \rangle$$

rewriting

$$\langle \psi | E_n | \psi \rangle = \frac{1}{2m} \langle \psi | p^2 | \psi \rangle + \frac{1}{2} m \omega^2 \langle \psi | x^2 | \psi \rangle - \frac{1}{2m \omega^2} \langle \psi | f^2 | \psi \rangle$$

since we know that

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$p = i \sqrt{\frac{m\hbar\omega}{2}} (-a + a^\dagger)$$

we have

$$\begin{aligned} \langle \psi | E_n | \psi \rangle &= -\frac{1}{2m} \left(\frac{m\hbar\omega}{2} \right) \langle \psi | -a^\dagger a + a^\dagger a^\dagger - a a^\dagger + a a | \psi \rangle \\ &\quad + \frac{1}{2m\omega^2} \left(\frac{\hbar}{2m\omega} \right) \langle \psi | a a + a a^\dagger + a^\dagger a + a^\dagger a^\dagger | \psi \rangle \\ &\quad - \frac{f^2}{2m\omega^2} \langle \psi | \psi \rangle \end{aligned}$$

where the creation and annihilation operator operates as

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle ; \quad a |n\rangle = \sqrt{n} |n-1\rangle$$

therefore $\langle \psi | E_n | \psi \rangle$ simplifies into

$$-\frac{\hbar\omega}{4} [-n - (n+1)] + \frac{\hbar\omega}{4} [n + n+1] - \frac{f^2}{2m\omega^2} = E_n$$

$$\frac{\hbar\omega}{4} (2n+1) + \frac{\hbar\omega}{4} (2n+1) - \frac{f^2}{2m\omega^2} = E_n$$

$$E_n = \frac{\hbar\omega(2n+1)}{2} - \frac{f^2}{2m\omega^2}$$

for the ground state energy we consider the value when $n=0$

$$E_0 = \frac{\hbar\omega}{2} - \frac{f^2}{2m\omega^2}$$

4.) For the first order correction of the ground state energy, we have

$$E_n^1 = \langle \psi_n^0 | H | \psi_n^0 \rangle$$

for the infinite square well we have

$$\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

therefore

$$E_n^1 = \langle \psi_n^0(x) | \alpha \delta(x - \frac{a}{2}) | \psi_n^0(x) \rangle$$

$$E_n^1 = \frac{2}{a} \alpha \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) \delta(x - \frac{a}{2}) dx$$

$$E_n^1 = \frac{2}{a} \alpha \sin^2\left(\frac{n\pi}{2}\right)$$

for the ground state energy for an infinite square well we have

$$E_1^1 = \frac{2}{a} \alpha$$

for the second order correction we have

$$E_n^2 = \sum_{n \neq l} \frac{|\langle \psi_l^0(x) | H | \psi_n^0(x) \rangle|^2}{E_n - E_l}$$

where

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$

therefore

$$E_n^2 = \sum_{n \neq l} \frac{\left| \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{n\pi x}{a}\right) \alpha \delta(x - \frac{a}{2}) dx \right|^2}{\frac{\hbar^2 \pi^2}{2ma^2} (n^2 - l^2)}$$

$$E_n^2 = \sum_{n \neq l} \frac{\frac{4}{a^2} \alpha^2 \sin^2\left(\frac{n\pi}{2}\right) \sin^2\left(\frac{l\pi}{2}\right)}{\frac{\hbar^2 \pi^2 (n^2 - l^2)}{2ma^2}}$$

$$E_n^2 = \sum_{n \neq l} \frac{8m\alpha^2}{\hbar^2 \pi^2 (n^2 - l^2)} \sin^2\left(\frac{n\pi}{2}\right) \sin^2\left(\frac{l\pi}{2}\right)$$

Again, since we are looking for groundstate corrections

$$E_0^2 = \sum_{l \neq 1} \frac{8m\alpha^2}{\hbar^2 \pi^2 (1 - l^2)} \sin^2\left(\frac{l\pi}{2}\right) = \begin{cases} 0, & l = \text{even} \\ \frac{8m\alpha^2}{\hbar^2 \pi^2 (1 - l^2)}, & l = \text{odd} \end{cases}$$