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P7.2.1 Consider $H' = \lambda x^4$ for the oscilator problem.

(i) Show that $E_n^1 = \frac{3\hbar^2\lambda}{4m^2\omega^2}[1+2n+2n^2]$

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$$H = H^0 + H^1 = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 + \lambda x^4$$

$$E_n^1 = \langle n^{(0)}|H'|n^{(0)}\rangle = \lambda\langle n^0|X^4|n^0\rangle$$ $|n^0\rangle$ is nth state of unperturbed operator

$$X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^+)$$ where $a^+|n\rangle = (n+1)^{1/2}|n+1\rangle$ and $a|n\rangle = n^{1/2}|n-1\rangle$

1
1 2 1
1 3 3 1
1 4 6 4 1

$$X^4 = \left(\frac{\hbar}{2m\omega}\right)^2(a+a^+)^4 = \left(\frac{\hbar}{2m\omega}\right)^2 \cancel{(a^4+4}((a+a^+)^2)^2$$

$$= \left(\frac{\hbar}{2m\omega}\right)^2(a^2+aa^+ + a^+a + a^{+2})^2$$

$$= \left(\frac{\hbar}{2m\omega}\right)^2(a^4 + a^2aa^+ + a^2a^+a + a^2a^{+2} + aa^+a^2 + aa^+aa^+ + aa^+a^+a + aa^+a^{+2}$$
$$+ a^+aa^2 + a^+aaa^+ + a^+aa^+a + \cancel{a^{+4}} + a^{+2}a^2 + a^{+2}aa^+ + a^{+2}a^+a + a^{+4})$$

for $\langle n^0|X^4|n^0\rangle$

$$X^4 = \left(\frac{\hbar}{2m\omega}\right)^2(a^2a^{+2} + aa^+aa^+ + aa^+a^+a + a^+aaa^+ + a^+aa^+a + a^{+2}a^2)$$ because the net effect of operators has to keep the same state $|n^0\rangle$

$$E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\langle n^0|a^2a^{+2} + aa^+aa^+ + aa^+a^+a + a^+aaa^+ + a^+aa^+a + a^{+2}a^2|n^0\rangle$$

$$E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\langle n^0|\{a^2a^+ + aa^+a + a^+aa\}(n^0+1)^{1/2}|n^0+1\rangle$$
$$+ \lambda\left(\frac{\hbar}{2m\omega}\right)^2\langle n^0|\{aa^{+2} + a^+aa^+ + a^{+2}a\}n^{1/2}|n-1\rangle$$

$$E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\{\langle n^0|a^2(n+2)^{1/2}(n+1)^{1/2}|n^0+2\rangle + \langle n^0|(aa^+ + a^+a)(n+1)^{1/2}(n+1)^{1/2}|n^0\rangle$$
$$+ \langle n^0|(aa^+ + a^+a)n^{1/2}(n^{1/2})|n^0\rangle + \langle n^0|a^{+2}n^{1/2}(n-1)^{1/2}|n-2\rangle$$

$$E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\{\langle n^0|a(n+2)^{1/2}(n+1)^{1/2}(n+2)^{1/2}|n+1\rangle + \langle n^0|a(n+1)^{1/2}(n+1)^{1/2}|n+1\rangle$$
$$+ \langle n^0|a^+(n+1)^{1/2}n^{1/2}|n-1\rangle + \langle n^0|an(n+1)^{1/2}|n+1\rangle + \langle n^0|a^+n\,n^{1/2}|n-1\rangle$$
$$+ \langle n^0|a^+(n-1)n^{1/2}|n-1\rangle\}$$

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

$$E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\{n^2+3n+2+n^2+2n+1+n^2+n+n^2+n+n^2+n^2-n\} = E_n^1 = \lambda\left(\frac{\hbar}{2m\omega}\right)^2\{6n^2+6n+3\}$$

17.2.1 (2) Argue that no matter how small λ is, the perturbation expansion will break down for some large enough n. What is the physical reason?

$E_n^0 = (n + 1/2)\hbar\omega$

1^{ST} order correction: $E_n^1 \propto n$

2^{ND} order correction: $E_n^2 \propto n^2$

for large n $\lim_{n\to\infty} E_n^{a} \propto n^{a} \to \infty$ and $\lim_{\substack{n\to\infty \\ m\to\infty}} E_n^m \propto n^m \to \infty$ fast!

The physical reason is that at high energy E_n $n\to\infty$, the particle has a larger $\langle x^2\rangle$ because $(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2)|E\rangle = E|E\rangle$ for unperturbed state $\Rightarrow$ a higher probability of higher values of x as $n\to\infty$ $\therefore$ λx^4 is no longer a small perturbation.

NOTE BOOK

Shankar 17.2.2 Consider a spin 1/2 particle with gyromagnetic ratio γ in a magnetic field $\vec{B} = B\hat{i} + B_0\hat{k}$. Treating B as a ~~perpendicular~~ perturbation, calculate the first- and second-order shifts in energy and first-order shift in wave function for the ground state. Then compare the exact answers expanded to the corresponding orders.

$$\hat{H} = \hat{H}^0 + \hat{H}^1 \qquad \hat{H}^0 = -\gamma B_0 \hat{S}_z \qquad \hat{H}^1 = -\gamma B \hat{S}_x$$

$$|+^0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \hat{H}|+^0\rangle = -\frac{\hbar\gamma B_0}{2}$$

$$|-^0\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \hat{H}|-^0\rangle = +\frac{\hbar\gamma B_0}{2}$$

$$E_+^{(1)} = \langle +^0|\hat{H}^1|+^0\rangle = -\gamma B\langle +^0|\hat{S}_x|+^0\rangle = 0$$

$$E_+^{(2)} = \sum_{i\neq +}^{\infty} \frac{|\langle i^{(0)}|\hat{H}^1|+^{(0)}\rangle|^2}{[E_+^{(0)} - E_i^{(0)}]} = \frac{|\langle -^{(0)}|\hat{H}^1|+^{(0)}\rangle|^2}{(E_+^{(0)} - E_-^{(0)})} \qquad i = \{+,-\}$$

$$E_+^{(2)} = \frac{(\gamma B)^2|\langle -^{(0)}|\hat{S}_x|+^{(0)}\rangle|^2}{(-\hbar\gamma B_0)} = \frac{(\gamma B)^2}{(-\hbar\gamma B_0)}\left|\left(\frac{1}{\sqrt{2}}\langle +_x^{(0)}| - \frac{1}{\sqrt{2}}\langle -_x^{(0)}|\right)\hat{S}_x\left(\frac{1}{\sqrt{2}}|+_x^{(0)}\rangle + \frac{1}{\sqrt{2}}|-_x^{(0)}\rangle\right)\right|^2$$

$$E_+^{(2)} = -\frac{\gamma B^2}{\hbar B_0}\left(\frac{1}{2}\right)^2\left\{\langle +_x^{(0)}|\hat{S}_x|+_x^{(0)}\rangle + \langle +_x^{(0)}|\hat{S}_x|-_x^{(0)}\rangle - \langle -_x^{(0)}|\hat{S}_x|-_x^{(0)}\rangle - \langle -_x^{(0)}|\hat{S}_x|+_x^{(0)}\rangle\right\}^2$$

$$E_+^{(2)} = -\frac{\gamma B^2}{4\hbar B_0}\left\{\frac{\hbar}{2} - \left(-\frac{\hbar}{2}\right)\right\}^2 = \frac{-\gamma B^2\hbar^2}{4\hbar B_0} = -\frac{\gamma B^2\hbar}{4B_0}$$

$$E_-^{(1)} = \langle -^0|\hat{H}^1|-^0\rangle = -\gamma B\langle -^0|\hat{S}_x|-^0\rangle = 0$$

$$E_-^{(2)} = \sum_{i\neq -}^{\infty} \frac{|\langle i^{(0)}|\hat{H}^1|-^{(0)}\rangle|^2}{(E_-^{(0)} - E_i^{(0)})} = \frac{|\langle +^{(0)}|\hat{H}^1|-^{(0)}\rangle|^2}{E_-^{(0)} - E_+^{(0)}} = \frac{(\gamma B)^2}{\hbar\gamma B_0}|\langle +^{(0)}|\hat{S}_x|-^{(0)}\rangle|^2, \quad i = \{+,-\}$$

$$E_-^{(2)} = \frac{\gamma B^2}{\hbar B_0}\left\{\left(\frac{1}{\sqrt{2}}\langle +_x^{(0)}| + \frac{1}{\sqrt{2}}\langle -_x^{(0)}|\right)\hat{S}_x\left(\frac{1}{\sqrt{2}}|+_x^{(0)}\rangle - \frac{1}{\sqrt{2}}|-_x^{(0)}\rangle\right)\right\}^2$$

$$E_-^{(2)} = \frac{\gamma B^2}{\hbar B_0}\left(\frac{1}{2}\right)^2\left\{\langle +_x^{(0)}|\hat{S}_x|+_x^{(0)}\rangle + \langle -_x^{(0)}|\hat{S}_x|+_x^{(0)}\rangle - \langle +_x^{(0)}|\hat{S}_x|-_x^{(0)}\rangle - \langle -_x^{(0)}|\hat{S}_x|-_x^{(0)}\rangle\right\}^2$$

$$E_-^{(2)} = \frac{\gamma B^2}{4\hbar B_0}\left\{\frac{\hbar}{2} - \left(-\frac{\hbar}{2}\right)\right\}^2 = +\frac{\gamma B^2\hbar}{4B_0}$$

$$\therefore E_+ = -\frac{\hbar\gamma B_0}{2} - \frac{\hbar\gamma B^2}{4B_0} \qquad E_- = +\frac{\hbar\gamma B_0}{2} + \frac{\hbar\gamma B^2}{4B_0}$$

$\Longrightarrow$

~~$|A\rangle = |A^{(0)}\rangle + \left(\frac{B}{2B_0}\right)^2 \ldots$~~

$$|+\rangle = |+_0\rangle + \frac{B}{2B_0}|-_0\rangle + \ldots$$

exact

$$|\vec{\sigma}_{\hat{n}}, \vec{S}_+\rangle = \begin{pmatrix} \cos\beta/2 \, e^{-i\alpha/2} \\ \sin\beta/2 \, e^{i\alpha/2} \end{pmatrix} \qquad \vec{n} = B_0 \hat{e}_z + B\vec{e}_x \Rightarrow \tan\beta = \frac{B}{B_0}$$

$$\vec{e}_n = \frac{\vec{n}}{|\vec{n}|} = \frac{B_0\vec{e}_x + B\vec{e}_z}{\sqrt{B_0^2 + B^2}}$$

$$E_0 = \frac{-\hbar\gamma}{2}\sqrt{B_0^2 + B^2} = \frac{\hbar\gamma}{2}B_0\left[1 + \frac{B^2}{2B_0^2} + \cancel{\ldots}\right]$$

$$= -\frac{\hbar\gamma B_0}{2} - \frac{\hbar\gamma}{2}\frac{B^2}{B_0}$$

$$|+\rangle = \cos\frac{\beta}{2}\begin{pmatrix} 1 \\ \tan\beta/2 \end{pmatrix} = \underbrace{\cos\frac{\beta}{2}}_{\to 1}\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix}\frac{B}{2B_0}\right]$$

$$= |+_0\rangle + \frac{B}{2B_0}|-^0\rangle + \ldots$$

17.2.3 In our study of the H atom, we assumed that the proton is a point charge e. This leads to the familiar Coulomb interaction $(-e^2/r)$ with the electron.

(1) Show that if the proton is a uniformly dense charge distribution of radius R, the interaction is

$$V = -\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3} \qquad r \le R$$

$$= -\frac{e^2}{r} \qquad r > R$$

let $\rho = \frac{e}{(4/3 \pi R^3)}$ be the uniform charge density for $r < R$

(Wangsness - Scalar Potential p.72) $r \to z$ since it is symmetric $\mu = \cos\theta'$

$$\phi = \frac{\rho}{4\pi\varepsilon_0} \int_0^{2\pi} \int_0^{\pi} \int_0^R \frac{r'^2 \sin\theta' dr' d\theta' d\varphi'}{(z^2 + r'^2 - 2zr' \cos\theta')^{1/2}} = \frac{\rho}{2\varepsilon_0} \int_0^R r'^2 dr' \int_{-1}^{+1} \frac{d\mu}{(z^2 + r'^2 - 2r'z\mu)^{1/2}}$$

$$-\frac{(z^2 + r'^2 - 2zr'\mu)^{1/2}}{zr'}\Bigg|_{-1}^{+1} = \frac{1}{zr'}\left(|z + r'| - |z - r'|\right)$$

1.) Outside the sphere $z > R$

let $z > 0 \Rightarrow r' \le R \quad z > r' \Rightarrow (z + r') - (z - r') = 2r' \Rightarrow$ integral over $\mu = 2/z$

$$\phi_0 = \frac{\rho R^3}{3\varepsilon_0 z} \quad \text{in Gaussian units} \Rightarrow \phi_0 = \frac{e}{4\pi\varepsilon_0 z} \Rightarrow \frac{e}{z}$$

2) Inside the sphere $z < R$

now r' can be $> r$ or $< r$

for $z < r' < R$

$$\frac{1}{zr'}\left[(z + r') - (r' - z)\right] = \frac{2}{r'}$$

for $r' < z < R$

$$\frac{1}{zr'}\left[(z + r') - (r' - z)\right] = \frac{2}{z}$$

$$\phi_i = \frac{\rho}{2\varepsilon_0}\left(\int_0^z r'^2 dr' \left(\frac{2}{z}\right) + \int_z^R r'^2 dr' \frac{2}{r'}\right) = \frac{\rho}{6\varepsilon_0}(3R^2 - z^2) = \frac{e}{4\pi\varepsilon_0}\left(\frac{3}{2R} - \frac{z^2}{2R^2}\right)$$

in Gaussian units

$$\phi_i = e\left(\frac{3}{2R} - \frac{z^2}{2R^2}\right)$$

$$V(r) = -e\,\phi(r)$$

$$\therefore \quad V(r) = -\frac{e^2}{r} \qquad r > R$$

$$= -\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3} \qquad r \le R$$

(2) Calculate ~~to~~ the first-order shift in the ground-state energy of the hydrogen due to this modification.

You may assume $e^{-R/a_0} \simeq 1$. You should find $E^1 = \frac{2e^2R^2}{5a_0^3}$

$$\hat{H} = \hat{H}^0 + \hat{H}^1$$

$$\hat{H}^0 = \frac{-e^2}{r} = V_0(r)$$

$$\hat{H}^1 = V(r) - V_0(r) = 0 \qquad r \geq R$$

$$\hat{H}^1 = -\frac{3e^2}{2R} + \frac{e^2r^2}{2R^3} + \frac{e^2}{r} \qquad r \leq R \checkmark$$

ground state Hydrogen atom $n=1$ $l=0$ $m=0$

~~$E_0^{(1)} = \langle v100|$~~

first order energy shift:

$$E_0^{(1)} = \langle 100|\hat{H}^1|100\rangle = 0 \quad r \geq R$$

$$E_0^{(1)} = \langle 100|\hat{H}^1|100\rangle = \langle 100|\left(\frac{3e^2}{2R} + \frac{e^2r^2}{2R^3} + \frac{e^2}{r}\right)|100\rangle \quad r \leq R$$

$$E_0^{(1)} = -\frac{3e^2}{2R}\langle 100|100\rangle + \frac{e^2}{2R^3}\langle 100|r^2|100\rangle + e^2\langle 100|\frac{1}{r}|100\rangle$$

$$\psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

$$\int_V \psi_{100}^* \psi_{100}\, d\tau = \left(\frac{1}{\pi a_0^3}\right) \int_0^{2\pi}\int_0^{\pi}\int_0^{R} e^{-2r/a_0} r^2 dr \sin\theta d\theta d\phi = \frac{4\pi}{\pi a_0^3}\int_0^R r^2 e^{-2r/a_0} dr$$

$$= \frac{4}{a_0^3}\left\{\frac{e^{-2r/a_0}}{(-2/a_0)}\right\}\left\{r^2 - \frac{2r}{(-2/a_0)} + \frac{2}{4/a_0^2}\right\}\Bigg|_0^R$$

$$= \frac{4}{a_0^3}\left(\frac{a_0}{2}\right)\left\{e^{-2R/a_0}\left[-R^2 - \cancel{2}Ra_0 - \frac{a_0^2}{2}\right] - e^0\left(-\frac{a_0^2}{2}\right)\right. \quad \left(e^{-2R/a_0} \sim 1\right)$$

$$= -\frac{2}{a_0^2}\left\{R^2 + Ra_0 + \cancel{\frac{a_0^2}{4}}\right\}$$

$$\int_V \psi_{100}^* \psi_{100} r^2 d\tau = \left(\frac{1}{\pi a_0^3}\right) 4\pi \int_0^R r^4 e^{-2r/a_0} dr$$

$$= \frac{4}{a_0^3} \frac{e^{-2r/a_0}}{(-2/a_0)} \left\{ r^4 - \frac{4r^3}{(-2/a_0)} + \frac{(4)(3)r^2}{(-2/a_0)^2} - \frac{(4)(3)(2)r}{(-2/a_0)^3} + \frac{(4)(3)(2)}{(-2/a_0)^4} \right\} \Bigg|_0^R$$

$$= \frac{-\cancel{2}\, e^{-2R/a_0}}{a_0^2} \left[R^4 + 2R^3 a_0 + 6R^2 a_0^2 + 12 R a_0^3 + \cancel{12 a_0^4} \right]$$

because $e^{-2R/a_0} = 1$
$-e^0 = 1$

$$= -\frac{2}{a_0^2} \left[R^4 + 2R^3 a_0 + 6R^2 a_0^2 + 12 R a_0^3 + \cancel{12 a_0^4} \right]$$

$$\int_V \psi_{100}^* \psi_{100} \frac{1}{r} \cancel{r^2} d\tau = \left(\frac{1}{\pi a_0^3}\right) 4\pi \int_0^R r e^{-2r/a_0} dr = \frac{4}{a_0^3} \frac{e^{-2r/a_0}}{(-2/a_0)} \left\{ r - \frac{1}{(-2/a_0)} \right\} \Bigg|_0^R$$

$$= \cancel{4}\; -\frac{2}{a_0^2} e^{-2R/a_0} \left\{ R + \frac{a_0}{2} \right\} + \frac{2}{a_0^2} e^0 \left\{ 0 + \frac{a_0}{2} \right\}$$

$$= \frac{-2}{a_0^2} R$$

$$E_0^{(1)} = -\frac{3e^2}{2R} \left\{ \frac{-2}{a_0^2} \left[R^2 + R a_0 \right] \right\} + \frac{e^2}{2R^3} \left\{ \frac{-2}{a_0^2} \left[R^4 + 2R^3 a_0 + 6R^2 a_0^2 + 12 R a_0^3 \right] \right\}$$

$$+ e^2 \left\{ \frac{-2R}{a_0^2} \right\}$$

$$E_0^{(1)} = \frac{3e^2 R}{a_0^2} - \frac{3e^2}{2a_0} \cancel{+} - \frac{e^2 R}{a_0^2} - \frac{e^2 2a_0}{a_0} - \frac{6e^2}{R} \cancel{+} - \frac{12 a_0}{R^2} - \frac{2e^2 R}{a_0^2}$$

$$E_0^{(1)} = \left(-\frac{3}{2} - 2 \right) \frac{e^2}{a_0} - \frac{6e^2}{R} - \frac{12 a_0}{R^2} = e^2 \left(\frac{-7}{2a_0} - \frac{6}{R} - \frac{12 a_0}{R^2} \right)$$

but this can't be correct because $a_0/R^2 \to \infty$? if $e^{-R/a_0} \to 1$???

trying again... $\hat{H}' = -\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3} + \frac{e^2}{r} \quad r \le R$

$$\psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0} \xrightarrow[r \ll a_0]{\lim} \left(\frac{1}{\pi a_0^3}\right)^{1/2} \qquad \int \psi_{100}^* \psi d\tau = \int_0^{2\pi} \int_0^{\pi} \int_0^R r^2 dr \sin\theta d\theta d\phi \left(\frac{1}{\pi a_0^3}\right) = \frac{4\pi}{a_0^3 \pi} \left(\frac{R^3}{3}\right)$$

$$E_0^{(1)} = \langle 100 | \hat{H}' | 100 \rangle = \langle 100 | \left(-\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3} + \frac{e^2}{r} \right) | 100 \rangle$$

$\Longrightarrow$

$$\int \psi_{100}^* \psi_{100}\, r^2\, d\tau = \oint \left(\frac{1}{\pi a_0^3}\right) \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^R r^4\, dr = \frac{4\pi}{\pi a_0^3}\left(\frac{R^5}{5}\right) = \frac{4}{5}\frac{R^5}{a_0^3} = \langle 100|r^2|100\rangle$$

$$\int \psi_{100}^* \psi_{100} \frac{1}{r}\, d\tau = \frac{1}{\pi a_0^3}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^R r\, dr = \frac{4\pi}{\pi a_0^3}\frac{R^2}{2} = \frac{2R^2}{a_0^3} = \langle 100|\tfrac{1}{r}|100\rangle$$

$$\int \psi_{100}^* \psi\, d\tau = \frac{4}{3}\frac{R^3}{a_0^3} = \langle 100|100\rangle$$

$$E_0^{(1)} = \langle 100|\left(-\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3} + \frac{e^2}{r}\right)|100\rangle \quad r \le R$$

$$E_0^{(1)} = \frac{-3e^2}{2R}\langle 100|100\rangle + \frac{e^2}{2R^3}\langle 100|r^2|100\rangle + e^2\langle 100|\tfrac{1}{r}|100\rangle$$

$$E_0^{(1)} = -\frac{3e^2}{2R}\left(\frac{4}{3}\frac{R^3}{a_0^3}\right) + \frac{e^2}{2R^3}\left(\frac{4}{5}\right)\frac{R^5}{a_0^3} + e^2\left(\frac{2R^2}{a_0^3}\right)$$

$$E_0^{(1)} = -\frac{e^2 2R^2}{a_0^3} + \frac{2e^2R^2}{5a_0^3} + \frac{e^2 2R^2}{a_0^3} = \frac{2}{5}\frac{e^2R^2}{a_0^3}$$

which is what Shankar tells us is the answer we should get.

?

$\Downarrow$

What is its numerical value?

17.2.4 (1) Prove the Thomas-Reiche-Kuhn sum rule

$$\sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle|^2 = \sum_{n'} (E_{n'} - E_n) \langle n|x|n'\rangle\langle n'|x|n\rangle = \frac{\hbar^2}{2m}$$

where $|n\rangle$ and $|n'\rangle$ are eigenstates of $\hat{H} = \hat{P}^2/2m + V(x)$.
Hint: Eliminate the $E_{n'} - E_n$ factor in favor of $\hat{H}$.)

$$\sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle|^2$$

$$= \sum_{n'} (E_{n'} - E_n) \langle n|x|n'\rangle\langle n'|x|n\rangle$$

$$= \sum_{n'} \left[\langle n|x|n'\rangle\langle n'|Hx|n\rangle - \langle n|Hx|n'\rangle\langle n'|x|n\rangle \right]$$

$$= \langle n|xHx|n\rangle - \langle n|Hxx|n\rangle = -\langle n|[Hx, x]|n\rangle = A$$

$$\sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle|^2$$

$$= \sum_{n'} (E_{n'} - E_n) \langle n|x|n'\rangle\langle n'|x|n\rangle$$

$$= \sum_{n'} \left[\langle n|x|n'\rangle\langle n'|Hx|n\rangle - \langle n|\cancel{Hx}^{\,x}|n'\rangle\langle n'|\cancel{x}^{\,xH}|n\rangle \right]$$

$$= \langle n|xHx|n\rangle - \langle n|xxH|n\rangle = -\langle n|[x, xH]|n\rangle = B$$

$$\sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle^2| = \frac{A+B}{2} = -\frac{1}{2}\left([HX, X] + [x, xH]\right) = -\frac{1}{2}\left([[H,x], x]\right)$$

$$[H, x] = \left[\frac{P^2}{2m}, X\right] + \cancel{[V(x), x]}^{\,0} = \frac{\hbar^2}{m}\frac{d}{dx}$$

$$[[H, x], x] = \frac{-\hbar^2}{m} \Rightarrow \frac{1}{2}([H, x], x]) = \frac{\hbar^2}{2m}$$

$$\therefore \sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle^2| = \frac{\hbar^2}{2m}$$

(2) test on n^{th} state of oscillator

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a^+ + a) \qquad E_n = (n + 1/2)\hbar\omega$$
$$E_{n'} - E_n = (n' - n)\hbar\omega$$

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n'|a^+ + a|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left[\langle n'|(n+1)^{1/2}|n+1\rangle \delta_{n', n+1} + \langle n'|n^{1/2}|n-1\rangle \delta_{n', n-1} \right]$$

$$\sum_{n'} (E_{n'} - E_n) |\langle n'|x|n\rangle^2| = \left(\frac{\hbar}{2m\omega}\right)\left[(E_{n+1} - E_n)(n+1) + (E_{n-1} - E_n)\, n\right] = \frac{\hbar}{2m\omega}(\hbar\omega)\left[(n+1-n)(n+1) - (n-1-n)n\right]$$

$$= \frac{\hbar^2}{2m} \quad //$$

Shankar 17.2.5 We have seen that if we neglect the repulsive e^2/r_{12} between the two electrons in the ground state of He, the energy is $-8Ry = -108.8eV$. Treating e^2/r_{12} as a perturbation, show that $\langle 100|\langle 100|H'|100\rangle|100\rangle = \frac{5}{2}R_y$. So that $E_0^0 + E_0^1 = -5.5R_y = -74.8eV$. (Recall that the measured value is $-78.6eV$ and the variational estimate is $-77.5eV$.)

Solution based on that in "Topics in Atomic Physics" by Charles E. Burkhardt Jacob L. Leventhal, Jacob Joseph Leventhal.

$$E_0^{(1)} = \langle n_0|\frac{1}{|\vec{r}_1-\vec{r}_2|}|n_0\rangle = {}_1\langle 100|{}_2\langle 100|\frac{1}{|\vec{r}_1-\vec{r}_2|}|100\rangle_1|100\rangle_2 = \int d\vec{r}_1 d\vec{r}_2 |\Psi_{1s}(\vec{r}_1)|^2 \frac{1}{|\vec{r}_1-\vec{r}_2|}|\Psi_{1s}(\vec{r}_2)|^2$$

ground state for one-electron atom $\Psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$ is independent of θ, ϕ

$\therefore \vec{r}_1 = r_1$

physically:

$|\Psi_{1s}(r_1)|^2 =$ probability of finding electron #1 at r_1

$|\Psi_{1s}(r_2)|^2 =$ charge density due to electron #2 at r_2

The integral over both is thus the electrostatic interaction energy of two overlapping spherically symmetric charge distributions.

Use ground state wave functions

$$E_0^{(1)} = \frac{Z^6}{\pi^2}\int dr_1 dr_2 \frac{1}{|\vec{r}_1-\vec{r}_2|} e^{-2Z(r_1+r_2)}$$

expand $\frac{1}{|\vec{r}_1-\vec{r}_2|}$ in terms of Legendre polynomials (Wagness)

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \frac{1}{r_1}\sum_{l=0}^{\infty}\left(\frac{r_2}{r_1}\right)^l P_l(\cos\theta) \quad r_1 > r_2$$

$$= \frac{1}{r_2}\sum_{l=0}^{\infty}\left(\frac{r_1}{r_2}\right)^l P_l(\cos\theta) \quad r_2 > r_1$$

where $\theta =$ angle between r_1 and r_2

use $\cos\theta = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2)$

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \frac{1}{r_1}\sum_{l=1}^{\infty}\frac{(r_<)^l}{(r_>)^{l+1}} P_l(\cos\theta) \quad \text{and} \quad P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^*(\theta_1\phi_1)Y_{lm}(\theta_2\phi_2)$$

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\frac{4\pi}{2l+1}\right)\frac{(r_<)^l}{(r_>)^{l+1}} Y_{lm}^*(\theta_1,\phi_1)Y_{lm}(\theta_2,\phi_2)$$

$$E_0^{(1)} = \frac{Z^6}{\pi^2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\frac{4\pi}{2l+1}\right)\int_0^{\infty} d^3r_1\, r_1^2 \int_0^{\infty} d^3r_2\, r_2^2\, e^{-2Z(r_1+r_2)}\frac{(r_<)^l}{(r_>)^{l+1}}\delta_{l,0}\delta_{m,0}$$

all terms vanish except $l = m = 0$

$$E_0^{(1)} = \frac{Z^6}{\pi^2} \cancel{\frac{1}{2}} \left(\frac{4\pi}{1}\right) \int_0^\infty d^3r_1 r_1^2 \int_0^\infty d^3r_2 r_2^2 \, e^{-Z(r_1+r_2)} \frac{1}{(r_>)}$$

$$\Rightarrow \quad E_0^{(1)} = \frac{5}{8} Z \qquad > 0$$

energy is raised by e-e repulsion

$$E_0 = E_0^{(0)} + E_0^{(1)} = -Z^2 + \frac{5}{8} Z = -74.8\,\text{eV}$$

experimentally : $E_0 - 79\,\text{eV}$

$\frac{5}{8}Z$ is significant fraction of $Z^2 = 4$

17.2.6 $\dfrac{2^{15} a_0^2}{3^{10}} = .55 a_0^2$

17.2.7 For oscillator, consider $H' = -qfX$. Find Ω that satisfies 17.2.38 → 17.2.39 for E_n^2 and compare with earlier calculation.

$$H' = [\Omega, H^0] \qquad H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$$

$$H' = \Omega H^0 - H^0 \Omega$$

$$-qfx = \Omega\frac{p^2}{2m} + \Omega\frac{m\omega^2x^2}{2} - \frac{p^2}{2m}\Omega - \frac{m\omega^2x^2}{2}\Omega$$

$$\cancel{= \Omega\frac{\hbar^2\partial^2}{2m\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Omega + \frac{\Omega m\omega^2x^2}{2} -}$$

$$= \Omega\left(\frac{\hbar^2\partial^2}{2m\partial x^2} + \frac{m\omega^2x^2}{2}\right) - \left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2x^2}{2}\right)\Omega = -qfx$$

$$\cancel{= \Omega\left(\frac{\hbar^2\partial^2}{2m\partial x^2} + \frac{m\omega^2x^2}{2}\right) \quad \Omega = e^{-\sqrt{qfx}}}$$

$$\cancel{= e^{\sqrt{qfx}}\left(\frac{p^2}{2m} + \frac{m\omega^2x^2}{2}\right) - qfx\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)e^{-\sqrt{qfx2m}/\hbar} - m\omega^2x^2e^{-\sqrt{qfx}} = -qfx}$$

$$\Omega = \left(e^{-\sqrt{qfx2m}/\hbar}\right)\ ?$$

-1

$$\Omega = (X+\delta) \quad \text{where } \delta = \frac{qf}{m\omega^2}$$

$$E_n^2 = \langle n^0|H'\Omega|n^0\rangle - \langle n^0|H'|n^0\rangle\langle n^0|\Omega|n^0\rangle$$

$$E_n^2 = \langle n^0|-qfx\left(\frac{qf}{m\omega^2}\right)|n^0\rangle - \langle n^0|-qfx|n^0\rangle\langle n^0|\frac{qf}{m\omega^2}|n^0\rangle$$

$$0 \qquad \frac{qf}{m\omega^2}\cancel{(n+\tfrac{1}{2})\hbar\omega}$$

$$\Omega = X+\delta \quad \delta = \frac{qf}{m\omega^2}$$

$$E_n^2 = \langle n^0|H'\Omega|n^0\rangle - \langle n^0|H'|n^0\rangle\langle n^0|\Omega|n^0\rangle$$

$$E_n^2 = \langle n^0|-qfX\left(X+\frac{qf}{m\omega^2}\right)|n^0\rangle - \langle n^0|-qfx|n^0\rangle\langle n^0|\left(X+\frac{qf}{m\omega^2}\right)|n^0\rangle$$

$$E_n^2 = -qf\langle n^0|x^2|n^0\rangle + \langle n^0|\frac{q^2f^2}{m\omega^2}x|n^0\rangle^{0}$$

$$E_n^2 = -qf\langle n^0|aa + a^\dagger a + aa^\dagger + a^\dagger a^\dagger|n^0\rangle = -qf\langle n^0|a^\dagger a + aa^\dagger|n^0\rangle$$

$$E_n^2 = -qf\langle n^0|n^{1/2}(n)^{1/2} + (n+1)^{1/2}(n+1)^{1/2}|n^0\rangle = -qf(n+n+1)\langle n^0|n^0\rangle =$$

$$= -qf(2n+1)$$

NOTE BOOK