SQ 6.

We use perturbation theory to estimate the relativistic correction to Hydrogen atom.

(1) The Hamiltonian is given by:

$$\hat{H} = \frac{p^2}{2m} + V(r) - \frac{p^4}{8m^3c^2},$$

here $V(r) = -\frac{e^2}{k_0 r}$

and $k_0 = 4\pi\varepsilon_0$

and the unperturbed term $\hat{H}_0 = \frac{p^2}{2m} + V(r)$,

which is the Hamiltonian of H-atom, with wavefunctions ψ_{nlm_l} and eigenenergies $E_n^{(0)} \sim -\frac{13.6}{n^2}\,eV$.

And the perturbation term $\hat{H}' = -\frac{p^4}{8m^3c^2}$ is the relativistic correction.

(2) We see that the relativistic term $\hat{H}'$ can

be related to $\hat{H}_0$ by:

$$\hat{H}' = -\frac{p^4}{8m^3c^2} = -\frac{1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 = -\frac{1}{2mc^2}\left[\hat{H}_0 - V(r)\right]^2$$

Then by 1st order perturbation theory,

$$E_{rel}^{(1)} = \langle \psi_{nlm}^{(0)} | \hat{H}' | \psi_{nlm}^{(0)} \rangle$$

$$= -\frac{1}{2mc^2} \langle \psi_{nlm}^{(0)} | \left(\hat{H}_0 + \frac{e^2}{k_0 r}\right)\left(\hat{H}_0 + \frac{e^2}{k_0 r}\right) | \psi_{nlm}^{(0)} \rangle$$

$$= -\frac{1}{2mc^2} \langle \psi_{nlm}^{(0)} | \hat{H}_0^2 + \frac{e^2}{k_0 r}\hat{H}_0 + \hat{H}_0\frac{e^2}{k_0 r} + \frac{e^4}{k_0^2 r^2} | \psi_{nlm}^{(0)} \rangle,$$

where $\langle \psi_{nlm}^{(0)} | \frac{e^2}{k_0 r}\hat{H}_0 | \psi_{nlm}^{(0)} \rangle = \langle \psi_{nlm}^{(0)} | \hat{H}_0 \frac{e^2}{k_0 r} | \psi_{nlm}^{(0)} \rangle$

$$= E_n^{(0)} \langle \psi_{nlm}^{(0)} | \frac{e^2}{k_0 r} | \psi_{nlm}^{(0)} \rangle$$

Then

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$$E_{rel}^{(1)} = -\frac{1}{2mc^2}\left[E_n^{(0)\,2} + 2E_n^{(0)}\frac{e^2}{k_0}\left\langle\frac{1}{r}\right\rangle + \frac{e^4}{k_0^2}\left\langle\frac{1}{r^2}\right\rangle\right].$$

(3) We directly apply the results

$$\left\langle\frac{1}{r}\right\rangle = \left\langle \psi_{nlm}^{(0)} \left| \frac{1}{r} \right| \psi_{nlm}^{(0)}\right\rangle = \frac{1}{n^2 a}$$

$$\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{(l+\frac{1}{2})n^3a^2},$$ where a is Bohr radius.

$$\Rightarrow E_{rel}^{(1)} = -\frac{1}{2mc^2}\left[E_n^{(0)2} + 2E_n^{(0)}\frac{e^2}{k_0}\frac{1}{n^2a} + \frac{e^4}{k_0^2}\frac{1}{(l+\frac{1}{2})n^3a^2}\right],$$

where $E_n^{(0)} = -\frac{1}{2}\left(\frac{e^2}{k_0\hbar}\right)^2\frac{m}{n^2}$, $a = \frac{k_0\hbar^2}{me^2}$

$$\Rightarrow E_{rel}^{(1)} = -E_n^{(0)}\left(\frac{E_n^{(0)}}{2mc^2}\right)\left\{1 - \frac{2}{\frac{1}{2}\left(\frac{e^2}{k_0\hbar}\right)^2\frac{m}{n^2}}\frac{e^2}{k_0}\frac{1}{n^2a}\right.$$

$$\left. + \frac{1}{\frac{1}{4}\left(\frac{e^2}{k_0\hbar}\right)^4\frac{m^2}{n^4}}\frac{e^4}{k_0^2}\frac{1}{(l+\frac{1}{2})n^3a^2}\right\}$$

$$= -E_n^{(0)}\left(\frac{E_n^{(0)}}{2mc^2}\right)\left\{\frac{4n}{l+\frac{1}{2}}-3\right\}$$

(4) We introduce the fine structure constant

$$\alpha = \frac{e^2}{k_0 \hbar c} \approx \frac{1}{137}.$$

The relativistic correction can be written as:

$$E_{rel}^{(1)} = -E_n^{(0)} \frac{1}{n^2} \alpha^2 \left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4} \right),$$

which is of order $\alpha^2 = \frac{1}{137^2} \approx 0.00006$.

i.e. $E_{rel}^{(1)} \sim 10^{-3}$ eV.

We see $E_{rel}^{(1)}$ is small comparing with $E_n^{(0)}$, and it generally depends on n and l.

sec 7.

(1) We have defined the creation and annihilation operators :

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right) \quad (1)$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right) \quad (2)$$

The commutator

$$[\hat{a}, \hat{a}^{+}] = \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a}$$

$$= \frac{m\omega}{2\hbar} \left(\hat{x}^2 - \frac{i}{m\omega} \hat{x}\hat{p} + \frac{i}{m\omega} \hat{p}\hat{x} + \frac{1}{m^2\omega^2} \hat{p}^2 \right)$$

$$- \frac{m\omega}{2\hbar} \left(\hat{x}^2 + \frac{i}{m\omega} \hat{x}\hat{p} - \frac{i}{m\omega} \hat{p}\hat{x} + \frac{1}{m^2\omega^2} \hat{p}^2 \right)$$

$$= -\frac{m\omega}{\hbar} \frac{i}{m\omega} [\hat{x}, \hat{p}]$$

$$= -\frac{1}{\hbar} \cdot i\hbar$$

$$= 1$$

(2) We express $\hat{H} = (\hat{a}^{+} a + \frac{1}{2})\hbar\omega$ as:

$$\hat{H} = \hbar\omega\left[\frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{i}{m\omega}[\hat{x}, \hat{p}] + \frac{1}{m^2\omega^2}\hat{p}^2\right) + \frac{1}{2}\right]$$

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

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

(3) We evaluate $\langle m|\hat{x}|n\rangle$ and $\langle m|\hat{p}|n\rangle$:

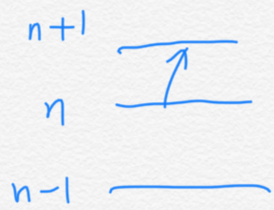
Firstly, from (1)(2), inversely we get

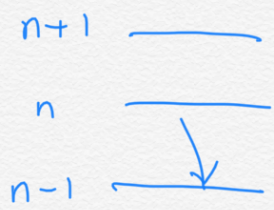
$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^{+} + \hat{a}\right)$$

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

Then $$\langle m|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle m|\,\hat{a}^{+} + \hat{a}\,|n\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\right)$$





This means that $\hat{x}$ only relates n state with (n-1) and (n+1) states.

$$\langle m|\hat{p}|n\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\,\langle m|\,\hat{a}^{+} - \hat{a}\,|n\rangle$$

$$= i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}\right),$$

where we have used the properties:

$$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle, \quad \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle,$$

and the orthonormal property of $|n\rangle$:

$$\langle m|n\rangle = \delta_{m,n}.$$

(4) We evaluate $\langle m|\hat{x}^2|n\rangle$ by inserting $\sum_j |j\rangle\langle j| = 1$,

$$\langle m|\hat{x}^2|n\rangle = \langle m|\hat{x}\sum_j |j\rangle\langle j|\hat{x}|n\rangle$$

$$= \frac{\hbar}{2m\omega}\sum_j \left(\sqrt{m}\,\delta_{j,m-1} + \sqrt{m+1}\,\delta_{j,m+1}\right)\left(\sqrt{n+1}\,\delta_{j,n+1} + \sqrt{n}\,\delta_{j,n-1}\right)$$

$$= \frac{\hbar}{2m\omega}\sum_j \Big[(n+1)\,\delta_{m,n}\,\delta_{j,n+1} + \sqrt{n(n-1)}\,\delta_{m,n-2}\,\delta_{j,n-1}$$

$$+ \sqrt{(n+1)(n+2)}\,\delta_{m,n+2}\,\delta_{j,n+1} + n\,\delta_{m,n}\,\delta_{j,n-1} \Big]$$

$$= \frac{\hbar}{2m\omega}\Big[(2n+1)\,\delta_{m,n} + \sqrt{n(n-1)}\,\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\,\delta_{m,n+2} \Big].$$