HOMEWORK 4 SOLUTIONS

15) So we need to calculate $\langle \phi_{1s}(1)\phi_{2s}(2) | \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|} | \phi_{2s}(1)\phi_{1s}(2)\rangle$

where

$$\phi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}$$

$$\phi_{2s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right) e^{-Zr/2a_0}$$

So when we put everything together we have

$$\Delta E = \frac{e^2}{4\pi\epsilon_0}\iint \rho_1(\vec{r}_1)\,\rho_2(\vec{r}_2)\,\frac{1}{|\vec{r}_1-\vec{r}_2|}\,d^3r_1\,d^3r_2$$

where $\rho_1=\rho_2 = \phi_{1s}(r)\phi_{2s}(r) = \frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3\left(\frac{1}{2}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right)e^{-3Zr/2a_0}$

We divide space into regions with $r_1 > r_2$ and $r_1 < r_2$. Then do the angular integrals (4π) for $d\Omega_1$ and (4π) for $d\Omega_2$. Then do the Gauss's Law trick to get

$$\Delta E = \frac{e^2}{4\pi\epsilon_0}(4\pi)^2\left\{\int_0^\infty \rho_2(r_2)\,\frac{1}{r_2}\left[\int_0^{r_2}\rho_1(r_1)\,r_1^2\,dr_1\right]r_2^2\,dr_2 \right.$$
$$\left. +\text{ a second identical term}\right\}$$

$$= \left(\frac{e^2}{4\pi\epsilon_0}\right)(4\pi)^2\left(\frac{1}{\pi}\right)^2\left(\frac{Z}{a_0}\right)^6\left(\frac{1}{8}\right)\overset{\text{(2 integrals)}}{(2)}\int_0^\infty\left(1-\frac{Zr_2}{2a_0}\right)e^{-3Zr_2/2a_0}$$
$$\times\frac{1}{r_2}\left[\int_0^{r_2}\left(1-\frac{Zr_1}{2a_0}\right)e^{-3Zr_1/2a_0}\,r_1^2\,dr_1\right]r_2^2\,dr_2$$

Lets do the inner integral. Let

$$x_1 = \frac{3Z}{2a_0}r_1 \qquad x_2 = \frac{3Z}{2a_0}r_2$$

$$[\,] = \int_0^{x_2}\left(1-\frac{1}{3}x_1\right)e^{-x_1}\left(\frac{2a_0}{3Z}\right)^3 x_1^2\,dx_1$$

$$= \left(\frac{2a_0}{3Z}\right)^3\left\{-(\cancel{x_1^2}+\cancel{2x_1}+\cancel{2})e^{-x_1}+\frac{1}{3}(x_1^3+\cancel{3x_1^2}+\cancel{6x_1}+\cancel{6})e^{-x_1}\right\}\Bigg|_0^{x_2}$$

$$= \left(\frac{2a_0}{3Z}\right)^3\left\{\frac{1}{3}x_2^3\,e^{-x_2}\right\}$$

So

$$\Delta E = 4\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{Z}{a_0}\right)^6 \int_0^\infty \left(1-\frac{Zr_2}{2a_0}\right) e^{-3Zr_2/2a_0}\frac{1}{r_2}$$

$$\times \left(\frac{\cancel{2a_0}}{\cancel{3Z}}\right)^3\left(\frac{1}{3}\right)\left(\frac{\cancel{3Z}}{\cancel{2a_0}}r_2\right)^3 e^{-3Zr_2/2a_0}\, r_2^2\, dr_2$$

$$= \frac{4}{3}\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{Z}{a_0}\right)^6 \int_0^\infty \left(1-\frac{Zr_2}{2a_0}\right) r_2^4\, e^{-3Zr_2/a_0}\, dr_2$$

Let

$$x = \frac{3Z}{a_0} r_2 \Rightarrow$$

$$\Delta E = \left(\frac{4}{3}\right)\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{Z}{a_0}\right)^6\left(\frac{a_0}{3Z}\right)^5 \int_0^\infty \left(1-\frac{x}{6}\right)x^4 e^{-x}\,dx$$

$$= \frac{4}{3}\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{Z}{a_0}\right)\left(\frac{1}{3}\right)^5\left[4! - \frac{1}{6}\cdot 5!\right]$$

$$= \frac{4}{3^6}\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{Z}{a_0}\left[24-20\right] = \boxed{\frac{2^4}{3^6}\,\frac{e^2}{4\pi\epsilon_0}\cdot\frac{Z}{a_0}}$$

1b) For $(1s)^1(2s)^1$ the starting energy (neglecting V_{ee}) is

$$E^{(0)} = -\frac{mc^2}{2}\alpha^2\left[\frac{Z^2}{(1)^2}+\frac{(Z)^2}{(2)^2}\right] = -\left[54.4\,eV + 13.6\,eV\right]$$

$$= -68.0\,eV$$

Then the corrections are

$$\Delta E^{(1)} = \Delta E_{DIR} \pm \Delta E_{EX}$$

$$= \left[\left(\frac{17}{81}\right) \pm \frac{2^4}{3^6}\right]\frac{e^2}{4\pi\epsilon_0}\cdot\frac{Z}{a_0} = [\;\;]\, Z mc^2\alpha^2$$

$$= 11.42\,eV \pm 1.19\,eV$$

$\Rightarrow$ we predict

$$E(^3s) = -68.0 + 11.42 - 1.19 = -57.77\,eV$$

$$E(^1s) = \;\;"\;\;\;\;"\;\; + 1.19 = -55.39\,eV.$$

17) $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ where $V(x) = \begin{cases} \infty & x<0 \\ Cx & x>0 \end{cases}$

$\psi_t = N x e^{-\alpha x}$ for $x>0$

Normalize

$$\langle \psi_t | \psi_t \rangle = N^2 \int_0^\infty x^2 e^{-2\alpha x}\, dx$$

Let $y = 2\alpha x$ $\quad dx = y/2\alpha$

$$\langle \psi_t | \psi_t \rangle = \frac{N^2}{(2\alpha)^3}\int_0^\infty y^2 e^{-y}\, dy = \frac{N^2}{(2\alpha)^3}\cdot 2 = 1$$

$$\boxed{N^2 = 4\alpha^3}$$

$E_t = \langle \psi_t | H | \psi_t \rangle$

$$\frac{d^2}{dx^2}\psi = N\frac{d}{dx}\left(e^{-\alpha x} - \alpha x e^{-\alpha x}\right) = N\left[-\alpha e^{-\alpha x} - \alpha e^{-\alpha x} + \alpha^2 x e^{-\alpha x}\right]$$

$$= \alpha N\left[\alpha x - 2\right] e^{-\alpha x}$$

So

$$E_t = -\frac{\hbar^2}{2m}\alpha N^2 \int_0^\infty x e^{-\alpha x}(\alpha x - 2) e^{-\alpha x}\, dx$$

$$+ C N^2 \int_0^\infty x e^{-\alpha x}\cdot x \cdot x e^{-\alpha x}\, dx$$

$$= N^2\left[-\frac{\hbar^2 \alpha}{2m}\int_0^\infty (\alpha x^2 - 2x) e^{-2\alpha x}\, dx\right.$$

$$\left. + C\int_0^\infty x^3 e^{-2\alpha x}\, dx\right]$$

Let $y = 2\alpha x \Rightarrow$

$$E_t = N^2\left[-\frac{\hbar^2\alpha}{2m}\int_0^\infty \left[\frac{y^2}{4\alpha} - 2\frac{y}{2\alpha}\right] e^{-y}\frac{dy}{2\alpha}\right.$$

$$\left. + C\int_0^\infty \left(\frac{1}{2\alpha}\right)^4 y^3 e^{-y}\, dy\right]$$

$$E_t = N^2 \left[-\frac{\hbar^2 \alpha}{2m}\left(\frac{1}{2\alpha}\right)\left(\frac{1}{4\alpha}\cdot 2 - \frac{1}{\alpha}\right)\right.$$

$$\left. + C\left(\frac{1}{2\alpha}\right)^4 \cdot 6 \right]$$

$\Rightarrow$

$$E_t = (4\alpha^3)\left[+ \frac{\hbar^2 \alpha}{2m}\left(\frac{1}{4\alpha^2}\right) + \frac{3}{8}\frac{C}{\alpha^4}\right]$$

$$= \frac{\hbar^2 \alpha^2}{2m} + \frac{3}{2}\frac{C}{\alpha}$$

Now choose α to minimize E_t.

$$\frac{dE_t}{d\alpha} = \cancel{2}\frac{\hbar^2 \alpha}{\cancel{2}m} - \frac{3}{2}\frac{C}{\alpha^2} = 0 \qquad \frac{\hbar^2 \alpha^3}{m} = \frac{3}{2}C$$

$$\alpha^3 = \frac{3}{2}\frac{Cm}{\hbar^2} \qquad \alpha = \left(\frac{3}{2}\frac{Cm}{\hbar^2}\right)^{\frac{1}{3}}$$

which gives

$$E_t = \frac{\hbar^2}{2m}\left(\frac{3}{2}\frac{Cm}{\hbar^2}\right)^{\frac{2}{3}} + \frac{3}{2}C\left(\frac{2}{3}\frac{\hbar^2}{Cm}\right)^{+\frac{1}{3}}$$

Lets combine the two terms

$$E_t = \frac{\hbar^2}{2m}\frac{3^{2/3}}{2^{2/3}}\frac{C^{2/3}m^{2/3}}{\hbar^{4/3}} + \frac{3}{2}C\left(\frac{2^{\frac{1}{3}}}{3^{1/3}}\right)\frac{\hbar^{2/3}}{C^{1/3}m^{1/3}}$$

$$= \frac{1}{2}\left(\frac{3}{2}\right)^{\frac{2}{3}}\frac{\hbar^{2/3}C^{\frac{2}{3}}}{m^{1/3}} + \left(\frac{3}{2}\right)^{\frac{2}{3}}\frac{\hbar^{2/3}C^{2/3}}{m^{1/3}}$$

$$= \left(\frac{3}{2}\right)\left(\frac{3}{2}\right)^{\frac{2}{3}}\frac{\hbar^{2/3}C^{2/3}}{m^{1/3}} = \boxed{\frac{3}{2}\left[\frac{9}{4}\frac{\hbar^2 C^2}{m}\right]^{\frac{1}{3}}}$$

18) The helium ground state energy is $-78.975\,eV$. According to the graph the wavelength to excite the $(2s)^1(2p)^1$ state is about $203.7\,\text{Å} = 20.37\,nm$ corresponding to

$$E = \frac{hc}{\lambda} = \frac{1240\,eV\cdot nm}{20.37\,nm} = 60.87\,eV$$

and so the state is at $E = -79.975 + 60.87 = -18.10\,eV$.

If the atom autoionizes to the ground state of He^+ the energy of the "atom" is $-54.4\,eV$ and so the emitted electron has (by energy conservation)

$$E = 54.4\,eV - 18.10\,eV = 36.3\,eV$$

$\Rightarrow$

$$\tfrac{1}{2} m v^2 = 36.3\,eV = E \qquad v = \left[2E/m\right]^{\frac{1}{2}} = \left[2E/mc^2\right]^{\frac{1}{2}} \cdot c$$

$$v = \left[\frac{2(36.3\,eV)}{5.11\times10^5\,eV}\right]^{\frac{1}{2}} \cdot c = 0.012\,c = \boxed{3.57\times10^6\ m/s}$$

If He^+ is in it's 1^{st} excited state the energy would be $-54.4\,eV/4 = -13.6\,eV$. This would require the emitted electron to have negative KE so <u>this decay does not occur.</u>

19) $$H = \frac{p^2}{2m} + \lambda x^4$$

We try

$$\psi_t = N e^{-\alpha x^2}$$

Normalize

$$\langle \psi_t | \psi_t \rangle = N^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx$$

$$= 2N^2 \int_0^{\infty} e^{-2\alpha x^2}\, dx$$

Using integral 666

$$\int_0^{\infty} x^{2n} e^{-ax^2}\, dx = \frac{1\cdot3\cdot5\cdots(2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}$$

$$\langle \psi_t | \psi_t \rangle = \frac{1}{2}\sqrt{\frac{\pi}{2\alpha}} \cdot 2N^2 = N^2 \sqrt{\frac{\pi}{2\alpha}} = 1 \Rightarrow N^2 = \sqrt{\frac{2\alpha}{\pi}}$$

$$\langle V \rangle = \langle \psi_t | V | \psi_t \rangle = \lambda \int_{-\infty}^{\infty} \psi_t^* x^4 \psi_t \, dx$$

$$= \lambda N^2 (2) \int_0^{\infty} x^4 e^{-2\alpha x^2} dx$$

$$= \lambda N^2 (2) \frac{1 \cdot 3}{8 (2\alpha)^2} \sqrt{\frac{\pi}{2\alpha}}$$

$$= 2\lambda \left(\frac{\cancel{2\alpha}}{\cancel{\pi}}\right)^{\frac{1}{2}} \frac{3}{32\alpha^2} \cancel{\sqrt{\frac{\pi}{2\alpha}}} = \frac{3}{16} \frac{\lambda}{\alpha^2}$$

$$\frac{p^2}{2m} \psi_t = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} N e^{-\alpha x^2} = -\frac{\hbar^2}{2m} N \frac{d}{dx} \left(-2\alpha x e^{-\alpha x^2}\right)$$

$$= -\frac{\hbar^2}{2m} N \left[-2\alpha e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2}\right]$$

$\Rightarrow$

$$\langle T \rangle = -\frac{\hbar^2}{2m} N^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(-2\alpha + 4\alpha^2 x^2\right) e^{-\alpha x^2} dx$$

$$= -\frac{\hbar^2}{2m} N^2 (2) \int_0^{\infty} -2\alpha \, e^{-2\alpha x^2} + 4\alpha^2 x^2 e^{-2\alpha x^2} dx$$

$$= -\frac{\hbar^2}{2m} \cancel{\sqrt{\frac{2\alpha}{\pi}}} (2) \left[-2\alpha \left(\frac{1}{2}\right) \cancel{\sqrt{\frac{\pi}{2\alpha}}} + 4\alpha^2 \frac{1}{4(2\alpha)} \cancel{\sqrt{\frac{\pi}{2\alpha}}}\right]$$

$$= -\frac{\hbar^2}{m} \left[-\alpha + \frac{\alpha}{2}\right] = +\frac{\hbar^2 \alpha}{2m}$$

$$E_t = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 \alpha}{2m} + \frac{3}{16} \frac{\lambda}{\alpha^2}$$

$$\frac{dE_t}{d\alpha} = \frac{\hbar^2}{2m} - \frac{3}{8} \frac{\lambda}{\alpha^3} = 0 \qquad \frac{\hbar^2}{2m} = \frac{3}{8} \frac{\lambda}{\alpha^3}$$

$$\alpha^3 = \frac{3}{4} \frac{\lambda m}{\hbar^2} \qquad \alpha = \left(\frac{3}{4}\right)^{\frac{1}{3}} \left(\frac{\lambda m}{\hbar^2}\right)^{\frac{1}{3}}$$

and so

$$E_t = \frac{\hbar^2}{2m} \left(\frac{3}{4}\right)^{\frac{1}{3}} \left(\frac{\lambda m}{\hbar^2}\right)^{\frac{1}{3}} + \frac{3}{16} \lambda \left(\frac{4}{3}\right)^{\frac{2}{3}} \left(\frac{\hbar^2}{\lambda m}\right)^{\frac{2}{3}}$$

$$E_t = \frac{1}{2}\left(\frac{3}{4}\right)^{\frac{1}{3}} \frac{\hbar^{\frac{4}{3}}\lambda^{\frac{1}{3}}}{m^{2/3}} + \frac{3}{16}\left(\frac{4}{3}\right)^{\frac{2}{3}} \frac{\hbar^{\frac{4}{3}}\lambda^{\frac{1}{3}}}{m^{2/3}}$$

$$= \left(\frac{1}{2}+\frac{1}{4}\right)\left(\frac{3}{4}\right)^{\frac{1}{3}}\left(\frac{\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}} = \left(\frac{3}{4}\right)^{\frac{4}{3}}\left(\frac{\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}$$

$$= \left[(3)^{4/3}/4\right] \lambda^{\frac{1}{3}}\left(\frac{\hbar^2}{2m}\right)^{\frac{2}{3}} = 1.0817\ \lambda^{\frac{1}{3}}\left(\frac{\hbar^2}{2m}\right)^{\frac{2}{3}}$$

So our trial wave function gives an energy too high by around 2%