Qm hw 4

vp1143

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(1)

(i)

Using the normalisation condition for $\psi_{nlm}(r,\theta,\phi)$,

$$\begin{aligned}1 = \int_V dV|\psi|^2 &= \int_0^\infty drr^2|R_{nl}(r)|^2 \int_\omega d\omega|Y_{lm}(\theta,\phi)|^2 \\ &= \int_0^\infty drr^2|R_{nl}(r)|^2 \\ &= \int_0^\infty dr\mathcal{P}_{nl}(r)\end{aligned}$$

Which gives, $\mathcal{P}_{nl}(r) = r^2|R_{nl}(r)|^2$.

(ii)

The radial probability density functions can be then expressed using table 4.7 as,

$$\mathcal{P}_{1s}(r) = r^2|R_{10}(r)|^2 = r^2 4a^{-3}\exp(\frac{-2r}{a}) \tag{1}$$

$$\mathcal{P}_{2s}(r) = r^2|R_{20}(r)|^2 = r^2\frac{1}{2}a^{-3}(1-\frac{r}{2a})^2\exp(\frac{-r}{a}) \tag{2}$$

$$\mathcal{P}_{2p}(r) = r^2|R_{21}(r)|^2 = r^2\frac{1}{24}a^{-3}(\frac{r}{a})^2\exp(\frac{-r}{a}) \tag{3}$$

Let $\rho = \frac{r}{a}$. Changing variable: $r \to \rho$,

$$\mathcal{P}_{1s}(r) = \frac{4\rho}{a}\exp(-2\rho) \tag{4}$$

$$\mathcal{P}_{2s}(r) = \frac{1}{2a}\rho^2(1-\frac{\rho}{2})^2\exp(-\rho) \tag{5}$$

$$\mathcal{P}_{2p}(r) = \frac{1}{24a}\rho^4\exp(-\rho) \tag{6}$$

The Figure 1 plot contains $a\mathcal{P}_{nl}(\rho)$ vs ρ,

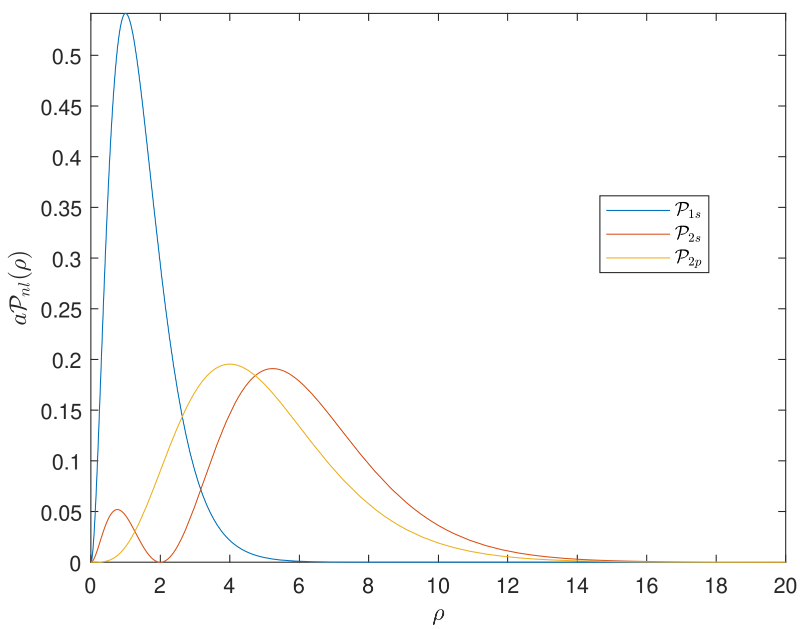

Figure 1: $a\mathcal{P}_{nl}(\rho)$ vs ρ

The expectation values for r^2 can be obtained using,

$$\langle r^2 \rangle_{nl} = \int_0^\infty dr r^2 \mathcal{P}_{nl}(r) = a^3 \int_0^\infty d\rho \rho^2 \mathcal{P}_{nl}(\rho) \tag{7}$$

Then using integration function in MATLAB,$\alpha = 8\pi\epsilon_0$

$$\sqrt{\langle r^2 \rangle_{1s}} = 0.4119\alpha$$
$$\sqrt{\langle r^2 \rangle_{2s}} = 1.54\alpha$$
$$\sqrt{\langle r^2 \rangle_{2p}} = 1.3025\alpha$$

An electron in $n = 1$ is closer to the centre of the Hydrogen atom than $n = 2$. The electron in $(2, 1)$ is closer to the centre than $(2, 0)$, because with lower angular momentum, classically, the electron has a highly eccentric orbit, thus spend more time away from the centre.

(iii)

$$\langle\Psi_0|V_{int}|\Psi_0\rangle = e^2\langle\Psi_0|\frac{1}{|\vec{r}_a - \vec{r}_b|}|\Psi_0\rangle \tag{8}$$

$$= e^2\int_{\Omega_a} d\Omega_a \int_{\Omega_b} d\Omega_b \int_0^\infty dr_a r_a^2 \int_0^\infty dr_b r_b^2 \psi_{100}(r_a)\psi_{100}(r_b)\frac{1}{|\vec{r}_a - \vec{r}_b|}\psi_{100}(r_a)\psi_{100}(r_b) \tag{9}$$

We can express $\frac{1}{|r_a - r_b|}$ using laplace expansion(Arfken,Weber),

$$\frac{1}{|r_a - r_b|} = \sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}\frac{\min(r_a,r_b)^l}{\max(r_a,r_b)^{l+1}}Y_{lm}^*(\theta_a,\phi_b)Y_{lm}(\theta_b,\phi_b) \tag{10}$$

For ease of notation call $Y_{lm}(\theta_a,\phi_a) = Y_{lm^a}$, same for b. Then using $\psi_{nlm} = R_{nl}Y_{mn}$, plugging (8) in (9), we have,

$$\int_{\Omega_a,\Omega_b} d\Omega_a d\Omega_b |Y_{00^a}|^2|Y_{00^b}|^2\sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}\frac{\min(r_a,r_b)^l}{\max(r_a,r_b)^{l+1}}Y_{lm^a}^*Y_{lm^b} \tag{11}$$

$$\times\iint_0^\infty dr_a dr_b r_a^2 r_b^2|R_{10^a}|^2|R_{10^b}|^2 \tag{12}$$

For the ease of notation let (12)$= I_r$. Using the fact that $Y_{00} = \frac{1}{2\sqrt{\pi}} = Y_{00}^*$, then we can say,

$$\frac{1}{4\pi}\sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}\frac{\min(r_a,r_b)^l}{\max(r_a,r_b)^{l+1}}\int_{\Omega_a,\Omega_b} d\Omega_a d\Omega_b Y_{00^a}Y_{lm^a}^*Y_{00^b}Y_{lm^b}I_r \tag{13}$$

$$\frac{1}{4\pi}\sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}\frac{\min(r_a,r_b)^l}{\max(r_a,r_b)^{l+1}}\delta_{0l}^2\delta_{0m}^2 I_r(\text{orthogonality}) \tag{14}$$

Let $l = 0$ and $m = 0$. Then (14) becomes,

$$\iint_0^\infty \frac{1}{\max(r_a,r_b)}dr_a dr_b r_a^2 r_b^2|R_{10^a}|^2|R_{10^b}|^2 \tag{15}$$

$$\tag{16}$$

Splitting integral into two $r_a > r_b$ and $r_a < r_b$ since there is a pole at $r_a = r_b$, and evaluating using Mathematica,

$$\int_0^\infty dr_a r_a^2|R_{10^a}|^2\left[\int_0^{r_a} dr_b r_b^2\frac{1}{r_a}|R_{10^b}|^2 + \int_{r_a}^\infty dr_b r_b|R_{10^b}|^2\right] \tag{17}$$

$$= 16a^{-6}\frac{5a^5}{128} = \frac{5}{8a} \tag{18}$$

Then,

$$\langle V_{int}\rangle = \frac{5}{8a}e^2 = \frac{5e}{8\times 4\pi\epsilon_0}eV \tag{19}$$

(2)

(i)

The degeneracy for Li ground state is $2\frac{1}{2}+1=2$. The complete wave functions for the two distinct states produced by the Slater determinant are,

$$\frac{1}{\sqrt{6}}\begin{vmatrix}\psi_{100}(r_1)|+\rangle & \psi_{100}(r_1)|-\rangle & \psi_{200}(r_1))|\pm\rangle \\ \psi_{100}(r_2)|+\rangle & \psi_{100}(r_2)|-\rangle & \psi_{200}(r_2))|\pm\rangle \\ \psi_{100}(r_3)|+\rangle & \psi_{100}(r_3)|-\rangle & \psi_{200}(r_3))|\pm\rangle\end{vmatrix} \tag{20}$$

$$= \frac{1}{\sqrt{6}}\psi_{100}(r_1)\psi_{100}(r_2)\psi_{200}(r_3)(|+-\pm\rangle - |-+\pm\rangle) \tag{21}$$

$$+\frac{1}{\sqrt{6}}\psi_{100}(r_1)\psi_{200}(r_2)\psi_{100}(r_3)(|-\pm+\rangle - |+\pm-\rangle) \tag{22}$$

$$+\frac{1}{\sqrt{6}}\psi_{200}(r_1)\psi_{100}(r_2)\psi_{100}(r_3)(|\pm+-\rangle - |\pm-+\rangle) \tag{23}$$

(ii)

The Energy of the Li ground state can be estimated by using the energy levels for Hydrogen and mulitplying it by $Z^2=9$,

$$E = 18E_1 + \frac{9}{4}E_1 = -13.6(20.25) = -275.4eV$$

We would need to evaluate three cross-potential expectation values,

$$e^2\langle 1s^2 2s|\frac{1}{|r_1-r_2|} + \frac{1}{|r_1-r_3|} + \frac{1}{|r_2-r_3|}|1s^2 2s\rangle \tag{24}$$

Which are all positive and thus, will increase the value of energy to a closer value to experimental.

(3)

(i)

$$n_e = \frac{9}{63.5} \times 6.023\times 10^{23} cm^{-3} = 8.5\times 10^{22} cm^{-3} = 8.5\times 10^{28} m^{-3}$$

(ii)

$$E_{Cu_F} = \frac{\hbar}{2m_e}(3\pi^2 n_e)^{\frac{2}{3}} = 7.049eV$$

$$T = 7.049 \times \frac{eV}{k_B} = 8.1\times 10^4 K$$

(iii)

The degeneracy pressure for Cu is,

$$P = \frac{2}{5} \times 8.5 \times 10^{28} \times 7.049 \times e = 3.83 \times 10^{10} Nm^{-2}$$

One Elephant weighs $6000kg$, the force exerted is $6000g = 6000 \times 9.81$, then the pressure in terms of elephant weight is,

$$\frac{3.83 \times 10^{10}}{6000 \times 9.81} = 5.26 \times 10^{7} Elephants/m^{2}$$

(4)

(a)

By equation 5.56,

$$E_{elec} = \frac{\hbar^2}{10\pi^2 m}(3\pi^2 Nd)^{\frac{5}{3}}(\frac{4\pi}{3}R^3)^{-\frac{2}{3}} = \frac{\hbar^2}{10\pi^2 mR^2}\frac{9}{2}(\frac{3}{2})^{\frac{1}{3}}\pi^{\frac{8}{3}}(dN)^{\frac{5}{3}} \tag{25}$$

(b)

By looking up on Wikipedia, the grtaviational energy for a uniformly dense sphere is,

$$U_G = -\frac{3}{5}\frac{GM_{tot}^2}{R} = -\frac{3}{5}\frac{GN^2M_{nucl}^2}{R} \tag{26}$$

(c)

Let $E(R) = \frac{a}{R^2}$ and $G = -\frac{b}{R}$. Minimising the total energy $H(R) = E_{elec}(R) + U_G(R)$ with respect to R,

$$H' = E'_{elec} + U'_G = -2aR^{-3} + bR^{-2} = 0 \Rightarrow R = \frac{2a}{b} \tag{27}$$

$$H'' = 6aR^{-4} - 2bR^{-3} \tag{28}$$

Substituting $R = \frac{2a}{b}$ in (28) we have,

$$H'' = 6a(\frac{2a}{b})^{-4} - 2b(\frac{2a}{b})^{-3} = \frac{b^4}{(2a)^3} > 0 \ as \ b^4 > 0 \tag{29}$$

Hence, it is a minima and we have,

$$R = \frac{2a}{b} = (\frac{9\pi}{4})^{\frac{2}{3}}\frac{\hbar^2 d^{\frac{5}{3}}}{GmM^2N^{\frac{1}{3}}} = (\frac{9\pi}{4})^{\frac{2}{3}}\frac{(6.62607004 \times 10^{-34})^2(\frac{1}{2})^{\frac{5}{3}}N^{-\frac{1}{3}}}{(6.674 \times 10^{-11})(9.1093 \times 10^{-31})(1.6726219 \times 10^{-27})^2}$$

$$= 7.6 \times 10^{25} N^{-\frac{1}{3}} m$$

(d)

Number of nucleons in the a white dwarf the size of sun can be given by,

$$N = \frac{M_\odot}{m_p} = \frac{1.98847 \times 10^{30}}{1.67 \times 10^{-27}} = 1.188 \times 10^{57}$$

. Then, $N^{\frac{1}{3}} = 1.0591 \times 10^{19}$. Using this,

$$R = \frac{7.6 \times 10^{25}}{1.0591 \times 10^{19}} = 7.16 \times 10^{6} m$$

(e)

Substituing R and N in (25),

$$E_F = 3.102 \times 10^{-14} J = \frac{3.102 \times 10^{-14}}{1.6 \times 10^{-19}} = 1.94 \times 10^{5} eV$$