

ADVANCED CHEMISTRY

QUANTUM MECHANICS H.W. - WINTER - WEEK 8

from the sheet

①
$$\begin{aligned} [\hat{L}^2, \hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x] \\ &= \underbrace{[\hat{L}_x^2, \hat{L}_x]}_0 + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] \\ &= [\hat{L}_y \cdot \hat{L}_y, \hat{L}_x] + [\hat{L}_z \cdot \hat{L}_z, \hat{L}_x] \\ &= \hat{L}_y [\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x] \hat{L}_y + \\ &\quad \hat{L}_z [\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x] \hat{L}_z \\ &= \hat{L}_y (-i\hbar \hat{L}_z) + (-i\hbar \hat{L}_z) \hat{L}_y + \hat{L}_z (i\hbar) \hat{L}_y \\ &\quad + (i\hbar \hat{L}_y) \hat{L}_z \\ &= -i\hbar \hat{L}_y \hat{L}_z - i\hbar \hat{L}_z \hat{L}_y + i\hbar \hat{L}_z \hat{L}_y + i\hbar \hat{L}_y \hat{L}_z \\ &= \underline{\underline{0}} \end{aligned}$$

$$\begin{aligned}
 (2) \quad R &= \frac{m_e e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \\
 &= \frac{(9.109 \times 10^{-31} \text{ kg})(1.602 \times 10^{-19} \text{ C})^4}{2(4\pi \times 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2})^2 (1.055 \times 10^{-34} \text{ Js})^2} \\
 &= 2.177144 \times 10^{-18} \frac{\text{kg C}^4}{\cancel{\text{C}^4} \text{ N}^{-2} \text{ m}^{-4} \text{ J}^2 \text{ s}^2} \\
 &= 2.177144 \times 10^{-18} \text{ J} \times \frac{1 \text{ eV}}{1.602 \times 10^{-19} \text{ J}} = \underline{\underline{13.59016 \text{ eV}}} \\
 &= \frac{1}{2} \text{ Hartree} = \underline{\underline{1 \text{ Rydberg}}} \\
 &\quad \text{2 Hartree}
 \end{aligned}$$

$$\begin{aligned}
 \text{or } 2.177144 \times 10^{-18} \text{ J} \times \left[\frac{1}{(6.626 \times 10^{-34} \text{ Js})(2.998 \times 10^{10} \text{ cm s}^{-1})} \right] \\
 = \underline{\underline{1.095983 \times 10^5 \text{ cm}^{-1}}}
 \end{aligned}$$

$$\begin{aligned}
 (3) \quad a_0 &= \frac{\hbar^2 (4\pi\epsilon_0)}{m_e e^2} = \frac{(1.055 \times 10^{-34} \text{ Js})^2 (4\pi \times 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2})}{(9.109 \times 10^{-31} \text{ kg})(1.602 \times 10^{-19} \text{ C})^2} \\
 &= 5.29735 \times 10^{-11} \frac{\text{J}^2 \text{ s}^2 \cancel{\text{C}^2} \text{ N}^{-1} \text{ m}^{-2}}{\text{kg } \cancel{\text{C}^2}} \quad \left(\frac{\text{N}^2 \text{ m}^2 \text{ s}^{-2} \text{ N}^{-1} \text{ m}^{-2}}{\text{kg}} \right) \\
 &= 5.29735 \times 10^{-11} \text{ m} \times \underline{\underline{10^{\circ} \text{ \AA}}} \quad \left(\frac{\text{Ns}^2}{\text{kg}} \frac{\text{kg m s}^{-2} \cdot \text{s}^2}{\cancel{\text{C}^2}} \right)
 \end{aligned}$$

$$\begin{aligned}
 \psi_{2p-1} + \psi_{2p+1} &= \frac{1}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \left[e^{-i\phi} + e^{i\phi} \right] \\
 &= \underbrace{\frac{1}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta}_A \left[\sin\phi - i\cos\phi + \sin\phi + i\cos\phi \right] \\
 &= 2A \sin\phi \\
 &= \frac{2}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \sin\phi
 \end{aligned}$$

$$\begin{aligned}
 \frac{1}{\sqrt{2}} \left[\psi_{2p-1} + \psi_{2p+1} \right] &= \frac{\sqrt{2}}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \sin\phi \\
 &= \frac{\sqrt{2}}{4 \times 2\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \sin\phi \\
 &= \frac{1}{4\sqrt{2\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \sin\phi \\
 &= \underline{\underline{\psi_{2py}}}
 \end{aligned}$$

$$\begin{aligned}
 \psi_{2p+1} - \psi_{2p-1} &= \frac{1}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \left[e^{i\phi} - e^{-i\phi} \right] \\
 &= \underbrace{\frac{1}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta}_A \left[\sin\phi + i\cos\phi - (\sin\phi - i\cos\phi) \right] \\
 &= A \left[2i\cos\phi \right]
 \end{aligned}$$

$$\frac{1}{i\sqrt{2}} \left[\psi_{2p+1} - \psi_{2p-1} \right] = \frac{2A}{\sqrt{2}} \cos\phi$$

$$= \frac{\sqrt{2}}{\sqrt{2}} \frac{1}{8\sqrt{\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \cos\phi$$

$$\frac{1}{i\sqrt{2}} \left(\psi_{2p_{+1}} - \psi_{2p_{-1}} \right) = \frac{1}{4\sqrt{2\pi}} \left(\frac{z}{a}\right)^{5/2} r e^{-zr/2a} \sin\theta \cos\phi$$

$$= \underline{\underline{\psi_{2p_x}}}$$

Chapter 10

③ $E = \frac{-\mu z^2 e^4}{2(4\pi\epsilon_0)^2 \hbar^2 n^2}$ for a H-like atom or ion

$$= \frac{-m_e e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \left(\frac{z}{n}\right)^2$$

$$\underbrace{\hspace{10em}}_{= R = 13.5902 \text{ eV}}$$

$$E = -(13.5902 \text{ eV}) \frac{z^2}{n^2} \quad \text{Ground state } n=1$$

$$\underline{\underline{\text{He}^+}} \quad E = -(13.5902 \text{ eV})(4) = \underline{\underline{-54.3608 \text{ eV}}}$$

$$\underline{\underline{\text{Li}^{2+}}} \quad E = -(13.5902 \text{ eV})(9) = \underline{\underline{-122.3118 \text{ eV}}}$$

$$\underline{\underline{\text{Be}^{3+}}} \quad E = -(13.5902 \text{ eV})(16) = \underline{\underline{-217.4432 \text{ eV}}}$$

$$\underline{\underline{\text{C}^{5+}}} \quad E = -(13.5902 \text{ eV})(36) = \underline{\underline{-489.2472 \text{ eV}}}$$

For the H atom $E = -(13.5902 \text{ eV}) \frac{1}{n^2}$ $Z=1$

(2)

(a) 3d orbital $n=3$

$$E = \underline{\underline{-1.5100 \text{ eV}}}$$

(b) 4f orbital, $n=4$ $E = \underline{\underline{-0.8494 \text{ eV}}}$

(c) 4p orbital $n=4$ $E = \underline{\underline{-0.8494 \text{ eV}}}$

(d) 6s orbital $n=6$ $E = \underline{\underline{-0.3775 \text{ eV}}}$

$$(4) \quad E = - \frac{\mu e^4 Z^2}{2(4\pi\epsilon_0)^2 \hbar^2 n^2} = - \frac{e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \left(\frac{\mu Z^2}{n^2} \right)$$

$$\begin{aligned} \frac{e^4}{2(4\pi\epsilon_0)^2 \hbar^2} &= \frac{(1.602 \times 10^{-19} \text{ C})^4}{2 \left[4\pi \times 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2} \right]^2 (1.055 \times 10^{-34} \text{ J s})^2} \\ &= 2.3901 \times 10^{12} \frac{\text{C}^4}{\text{N}^{-2} \text{ m}^{-4} \text{ J}^2 \text{ s}^2} \\ &= 2.3901 \times 10^{12} \text{ m}^2 \text{ s}^{-2} \end{aligned}$$

$$E = - \left(2.3901 \times 10^{12} \text{ m}^2 \text{ s}^{-2} \right) \left(\frac{\mu Z^2}{n^2} \right) \quad \begin{aligned} &= \frac{\text{N}^2 \text{ m}^4}{\text{N}^2 \text{ m}^2 \text{ s}^2} \\ &= \text{m}^2 \text{ s}^{-2} \end{aligned}$$

$$\mu_H = \frac{m_N \cdot m_e}{m_N + m_e} = \frac{(1.673 \times 10^{-27}) (9.109 \times 10^{-31}) \text{ kg}}{(1.673 \times 10^{-27} + 9.109 \times 10^{-31})}$$

$$\mu_H = 9.1040 \times 10^{-31} \text{ kg}$$

For the deuterium atom the nucleus contains a proton and a neutron.

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$$\mu_D = \frac{(m_p + m_n) m_e}{(m_p + m_n) + m_e}$$

$$= \frac{(1.673 \times 10^{-27} + 1.675 \times 10^{-27}) 9.109 \times 10^{-31} \text{ kg}}{(1.673 \times 10^{-27} + 1.675 \times 10^{-27} + 9.109 \times 10^{-31})}$$

$$\mu_D = 9.1065 \times 10^{-31} \text{ kg}$$

$$E_H = - (2.3901 \times 10^{12} \text{ m}^2 \text{ s}^{-2}) (9.1040 \times 10^{-31} \text{ kg}) \frac{1}{2}$$

$$E_H = - 2.1759 \times 10^{-18} \text{ J}$$

$$E_D = - (2.3901 \times 10^{12} \text{ m}^2 \text{ s}^{-2}) (9.1065 \times 10^{-31} \text{ kg}) \frac{1}{2}$$

$$= - 2.1765 \times 10^{-18} \text{ J}$$

Ionization potential of H = $\underline{\underline{2.1759 \times 10^{-18} \text{ J}}}$

of D = $\underline{\underline{2.1765 \times 10^{-18} \text{ J}}}$

For H

$$E_{n_1} = - 2.1759 \times 10^{-18} \frac{\text{J}}{n_1^2} \quad E_{n_2} = - 2.1759 \times 10^{-18} \frac{\text{J}}{n_2^2}$$

$$\frac{\Delta E}{hc} = \frac{1}{\lambda} = \frac{E_2 - E_1}{hc} = \frac{2.1759 \times 10^{-18} \text{ J}}{(6.626 \times 10^{-34} \text{ Js})(2.99 \times 10^8 \text{ m s}^{-1})} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$$= 1.0983 \times 10^7 \text{ m}^{-1} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

For the Balmer series first line $n_1 = 2$ $n_2 = 3$

$$\frac{1}{\lambda} = 1.0983 \times 10^7 \text{ m}^{-1} \left[\frac{1}{4} - \frac{1}{9} \right] = 1.5254 \times 10^6 \text{ m}^{-1}$$

$$\lambda = 6.5557 \times 10^{-7} \text{ m} = \underline{\underline{655.57 \text{ nm}}}$$

For D

$$E_{n_1} = -2.1765 \times 10^{-18} \frac{\text{J}}{n_1^2} \quad E_{n_2} = -2.1765 \times 10^{-18} \frac{\text{J}}{n_2^2}$$

$$\frac{1}{\lambda} = \frac{2.1765 \times 10^{-18}}{(6.626 \times 10^{-34} \text{ Js})(2.99 \times 10^8 \text{ m s}^{-1})} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

For the Balmer series, first line $n_1 = 2$ $n_2 = 3$

$$\frac{1}{\lambda} = 1.5258 \times 10^6 \text{ m}^{-1}$$

$$\lambda = 6.5538 \times 10^{-7} \text{ m} = \underline{\underline{655.38 \text{ nm}}}$$

⑥

$$\mu = \frac{m_p m_{\text{muon}}}{m_p + m_{\text{muon}}} = \frac{(1.673 \times 10^{-27} \text{ kg})(200 \times 9.109 \times 10^{-31} \text{ kg})}{[1.673 \times 10^{-27} + (200 \times 9.109 \times 10^{-31})] \text{ kg}}$$

$$\mu = \underline{\underline{1.6429 \times 10^{-28} \text{ kg}}}$$

$$R = \frac{\mu e^4}{2(4\pi\epsilon_0)^2 h^2}$$

Where e = charge of muon

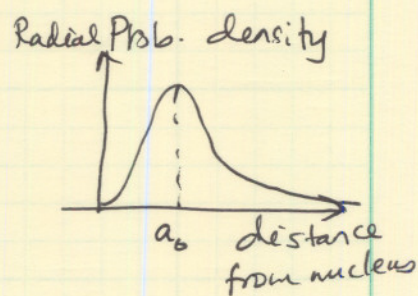
μ = reduced mass of muon^M atom

$$R = \frac{(1.6429 \times 10^{-28} \text{ kg})(1.602 \times 10^{-19} \text{ C})^4}{2(4\pi \times 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2})^2 (1.055 \times 10^{-34} \text{ Js})^2}$$

$$= \underline{\underline{3.9267 \times 10^{-16} \text{ J}}}$$

$$E = \frac{-\mu e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \left(\frac{Z^2}{n^2} \right) = \underline{\underline{-R \frac{Z^2}{n^2}}}$$

most probable radius } = a_0
for a 1s orbital



$$a_0 = \frac{\hbar^2 (4\pi\epsilon_0)}{m_{\text{muon}} e^2} \quad e = \text{charge of muon}$$

$$a_0 = \frac{(1.055 \times 10^{-34} \text{ Js})^2 (4\pi \times 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2})}{(200 \times 9.109 \times 10^{-31} \text{ kg})(1.602 \times 10^{-19} \text{ C})^2}$$

$$= 2.6488 \times 10^{-13} \text{ m} \times \frac{10^2 \text{ pm}}{\text{m}} = \underline{\underline{0.26488 \text{ pm}}}$$

③ $\frac{1}{\lambda} = R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$ Paschen series

$n_1 = 3$ $n_2 = 4, 5, 6$

for the first three lines

$$\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1} \left[\frac{1}{9} - \frac{1}{16} \right]$$

$$= 5.3326 \times 10^5 \text{ m}^{-1}$$

$$\lambda = 1.87524 \times 10^{-6} \text{ m} = \underline{\underline{1.87524 \mu\text{m}}}$$

$$\left(10^{-6} \text{ m} = 1 \mu\text{m} \right)$$

For the second line

$$\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1} \left(\frac{1}{9} - \frac{1}{25} \right) = 7.8009 \times 10^5 \text{ m}^{-1}$$

$$\lambda = 1.28191 \times 10^{-6} \text{ m} = \underline{\underline{1.28191 \mu\text{m}}}$$

Third line $\frac{1}{\lambda} = 1.097 \times 10^7 \text{ m}^{-1} \left(\frac{1}{9} - \frac{1}{36} \right) = 9.14167 \times 10^5 \text{ m}^{-1}$

$$\lambda = 1.09389 \times 10^{-6} \text{ m} = \underline{\underline{1.09389 \mu\text{m}}}$$

⑨

$$\frac{1}{\lambda} = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_2 > n_1$$

$$n_2 = 100 \quad n_1 = 99$$

$$= 1.097 \times 10^7 \text{ m}^{-1} \left[\frac{1}{99^2} - \frac{1}{100^2} \right]$$

$$= 22.27354 \text{ m}^{-1}$$

$$\lambda = 4.48963 \times 10^{-2} \text{ m} = \underline{\underline{4.48963 \text{ cm}}}$$

⑩

$$R = \frac{\mu e^4}{2(4\pi\epsilon_0)^2 \hbar^2} = A(\text{say}) = \mu A$$

When the nucleus is extremely heavy

$$\mu = \frac{m_e m_N}{m_e + m_N} = \frac{m_N \cdot m_e}{m_N} = m_e$$

\therefore When the nucleus is extremely heavy

$$R_\infty = \mu A = m_e A$$

$$\text{for H atom } R_H = \mu_H A$$

$$\frac{R_H}{R_\infty} = \frac{\mu_H A}{m_e A} = \frac{\mu_H}{m_e} = \frac{1}{m_e} \left[\frac{m_e \cdot m_N}{m_e + m_N} \right]$$

$$= \frac{m_N}{m_e + m_N}$$

$$R_H = R_\infty \left(\frac{m_N}{m_e + m_N} \right)$$

$$R_H = 10973731.534 \text{ m}^{-1} \left[\frac{1.673 \times 10^{-27} \text{ kg}}{9.109 \times 10^{-31} \text{ kg} + 1.673 \times 10^{-27} \text{ kg}} \right]$$

$$= \underline{\underline{1.0967759 \times 10^7 \text{ m}^{-1}}}$$

$$R_D = R_\infty \left(\frac{m_N}{m_e + m_N} \right)$$

$$= 10973731.534 \text{ m}^{-1} \left[\frac{(1.673 \times 10^{-27} + 1.675 \times 10^{-27}) \text{ kg}}{(9.109 \times 10^{-31} + 1.673 \times 10^{-27} + 1.675 \times 10^{-27}) \text{ kg}} \right]$$

$$R_D = \underline{\underline{1.0970747 \times 10^7 \text{ m}^{-1}}}$$

$$(11) \quad \psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0} \right)^{3/2} e^{-zr/a_0}$$

$$\int \psi_{100}^* \psi_{100} d\tau = \int \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0} \right)^{3/2} e^{-zr/a_0} \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0} \right)^{3/2} e^{-zr/a_0} d\tau$$

$$= \frac{1}{\pi} \left(\frac{z}{a_0} \right)^3 \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-2zr/a_0} r^2 \sin\theta dr d\theta d\phi$$

$$= \frac{1}{\pi} \left(\frac{z}{a_0} \right)^3 \int_0^{\infty} e^{-2zr/a_0} r^2 dr \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi$$

$$= \frac{1}{\pi} \left(\frac{z}{a_0} \right)^3 \int_0^{\infty} r^2 e^{-2zr/a_0} dr \left[(-\cos\theta) \Big|_0^{\pi} (\phi) \Big|_0^{2\pi} \right]$$

$$= \frac{1}{\pi} \left(\frac{z}{a_0} \right)^3 \left[\frac{2!}{\left(\frac{2z}{a_0} \right)^3} \right] (-\cos\pi + \cos 0) (2\pi)$$

$$\int_0^{\infty} x^n e^{-kx} dx = \frac{n!}{k^{n+1}}$$

$$= \left(\frac{1}{\pi} \right) \left(\frac{z}{a_0} \right)^3 \left(\frac{a_0}{2z} \right)^3 2(1+1)(2\pi) = \cancel{8} \left(\frac{z^3}{a_0^3} \right) \left(\frac{a_0^3}{\cancel{8} z^3} \right) = \underline{\underline{1}}$$

$\therefore \psi_{100}$ is normalized.

$$(12) \int \psi_{100}^* \psi_{200} d\tau = \int \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0} \right)^{3/2} e^{-zr/a_0} \frac{1}{4\sqrt{2}\pi} \left(\frac{z}{a_0} \right)^{3/2} \left(2 - \frac{zr}{a_0} \right) e^{-zr/2a_0} d\tau$$

$$= \frac{1}{4\sqrt{2}(\pi)^{3/2}} \left(\frac{z}{a_0} \right)^3 \int \left(2 - \frac{zr}{a_0} \right) e^{-3zr/2a_0} d\tau$$

$$= \frac{1}{4\sqrt{2}(\pi)^{3/2}} \left(\frac{z}{a_0} \right)^3 \int \left(2 - \frac{zr}{a_0} \right) e^{-3zr/2a_0} r^2 dr \sin\theta d\theta d\phi$$

$$= \frac{1}{4\sqrt{2}(\pi)^{3/2}} \left(\frac{z}{a_0} \right)^3 \int_0^r \left(2r^2 - \frac{zr^3}{a_0} \right) e^{-3zr/2a_0} dr \underbrace{\int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi}_{=(4\pi)}$$

$$\begin{aligned}
&= \frac{1}{4\sqrt{2}(\pi)^{3/2}} \left(\frac{z}{a_0}\right)^3 \left[2 \int_0^{\infty} r^2 e^{-3zr/2a_0} dr - \left(\frac{z}{a_0}\right) \int_0^{\infty} r^3 e^{-3zr/2a_0} dr \right] (4\pi) \\
&= \underbrace{\frac{1}{4\sqrt{2}(\pi)^{3/2}}}_{A''} \left[2 \frac{2!}{\left(\frac{3z}{2a_0}\right)^3} - \left(\frac{z}{a_0}\right) \frac{3!}{\left(\frac{3z}{2a_0}\right)^4} \right] (4\pi) \\
&= 4\pi A \left[4 \frac{8a_0^3}{27z^3} - \frac{z}{a_0} \cdot \frac{6 \cdot 16a_0^4}{81z^4} \right] \\
&= 4\pi A \left[\frac{32a_0^3}{27z^3} - \frac{32a_0^3}{27z^3} \right] = 0
\end{aligned}$$

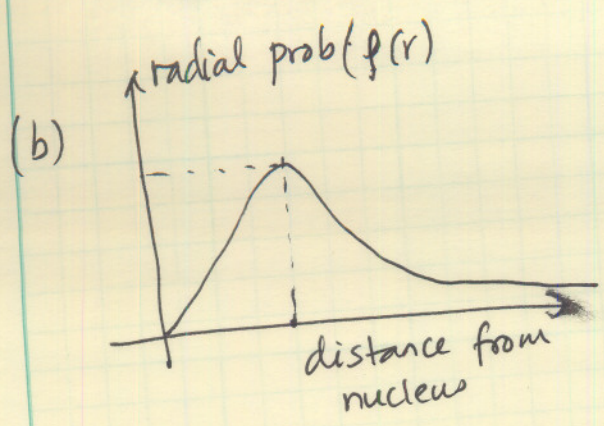
$\therefore \psi_{100}$ and ψ_{200} are orthogonal.

(13) (a) $\langle r \rangle = \int \psi_{100}^* r \psi_{100} d\tau$

$$\begin{aligned}
&= \int \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0} r \frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0} d\tau \\
&= \frac{1}{\pi} \left(\frac{z}{a_0}\right)^3 \iiint e^{-2zr/a_0} r \cdot r^2 dr \sin\theta d\theta d\phi \\
&= \frac{1}{\pi} \left(\frac{z}{a_0}\right)^3 \int_0^{\infty} r^3 e^{-2zr/a_0} dr \underbrace{\int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi}_{= 4\pi}
\end{aligned}$$

$$= \frac{1}{\pi} \left(\frac{z}{a_0}\right)^3 \left[\frac{3!}{\left(\frac{2z}{a_0}\right)^4} \right] (4\pi) = \frac{z^3}{a_0^3} \cdot \frac{6 \cdot a_0^4 \cdot 4}{16 z^4}$$

$$= \frac{24 a_0}{16 z} = \underline{\underline{\frac{3}{2z} a_0}}$$



Radial probability = $4\pi r^2 [R_{nl}(r)]^2 = f(r)$

at the most probable value of r , there is a maximum in the radial probability $f(r)$.

\therefore at the most probable value of r ,

$$\frac{df(r)}{dr} = 0$$

$f(r)$ for 1s orbital = $4\pi r^2 R_{10}(r)$

$$= 4\pi r^2 \left[\frac{1}{\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0} \right]^2$$

$$f(r) = \left(4\sqrt{\pi} \left(\frac{z}{a_0}\right)^{3/2} r^2 e^{-zr/a_0} \right)^2$$

$$\frac{df(r)}{dr} = \frac{d}{dr} \left[\underbrace{4\sqrt{\pi} \left(\frac{z}{a_0}\right)^{3/2}}_{=A} r^2 e^{-zr/a_0} \right]^2$$

$$f(r) = 4\pi r^2 \left(\frac{1}{\pi}\right) \left(\frac{z}{a_0}\right)^3 e^{-2zr/a_0}$$

$$= 4\pi \left(\frac{z}{a_0}\right)^3 r^2 e^{-2zr/a_0}$$

$$\frac{df(r)}{dr} = 4 \left(\frac{z}{a_0}\right)^3 \frac{d}{dr} \left[r^2 e^{-2zr/a_0} \right] = 0$$

$$= 4 \left(\frac{z}{a_0}\right)^3 \left[2r e^{-2zr/a_0} + r^2 \left(-\frac{2z}{a_0}\right) e^{-2zr/a_0} \right] = 0$$

$$r e^{-2zr/a_0} \left[2 - \frac{2zr}{a_0} \right] = 0 \quad r \neq e^{-2zr/a_0} \neq 0$$

$$\Rightarrow \left[2 - \frac{2zr}{a_0} \right] = 0 \Rightarrow r = \frac{a_0}{z}$$

$$r = a_0/z$$

∴ most probable distance $(r) = \underline{\underline{a_0/z}}$