Date..............

MS 50023

Assignment 2

Q.1

Soln Water molecule consists of two H atoms (H1, H2) and one O atom (O).
Let's denote nuclei of H1 with I, nuclei of H2 with J and nuclei of O with k.
Let's denote all the electrons with i.

$$\hat{H}_{H_2O} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_I \frac{1}{2M_I}\nabla_I^2 - \sum_J \frac{1}{2M_J}\nabla_J^2$$
$$-\sum_k \frac{1}{2M_k}\nabla_k^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J}{|R_I - R_J|} + \frac{1}{2}\sum_{J\neq K}\frac{Z_J Z_K}{|R_J - R_K|}$$
$$+\frac{1}{2}\sum_{I\neq K}\frac{Z_I Z_K}{|R_I - R_K|} + \frac{1}{2}\sum_{i\neq j}\frac{1}{|r_i - r_j|}$$
$$-\sum_{i,I}\frac{Z_I}{|r_i - R_I|} - \sum_{i,J}\frac{Z_J}{|r_i - R_J|} - \sum_{i,K}\frac{Z_K}{|r_i - R_K|}$$

Apply clamped ion approximation and substitute
$Z_I = 1,\ Z_J = 1,\ Z_K = 8$

$$\hat{H}_{H_2O} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{1}{|r_i - r_j|} - \sum_{i,I}\frac{1}{|r_i - R_I|}$$
$$-\sum_{i,J}\frac{1}{|r_i - R_J|} - \sum_{i,K}\frac{8}{|r_i - R_K|}$$

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Spiral

Q.3

Soln He atom

$$\psi(r_1, r_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(r_1) & \psi_2(r_2) \\ \psi_2(r_1) & \psi_1(r_2) \end{vmatrix}$$

$$= \frac{1}{\sqrt{2}} \left(\psi_1(r_1)\psi_1(r_2) - \psi_2(r_1)\psi_2(r_2) \right)$$

$$n(r) = 2 \int |\psi(r, r_2)|^2 \, dr_2$$

$$= 2 \int \psi(r, r_2)\, \psi^*(r, r_2)\, dr_2$$

$$= 2 \cdot \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \int \left(\psi_1(r)\psi_1(r_2) - \psi_2(r)\psi_2(r_2) \right) \left(\psi_1^*(r)\psi_1^*(r_2) - \psi_2^*(r)\psi_2^*(r_2) \right) dr_2$$

$$= \int \left(|\psi_1(r)|^2 |\psi_1(r_2)|^2 + |\psi_2(r)|^2 |\psi_2(r_2)|^2 - \psi_1^*(r)\psi_2(r)\psi_1^*(r_2)\psi_2(r_2) - \psi_1(r)\psi_2^*(r) \times \psi_1(r_2)\psi_2^*(r_2) \right) dr_2$$

$$= |\psi_1(r)|^2 \int |\psi_1(r_2)|^2 dr_2 + |\psi_2(r)|^2 \int |\psi_2(r_2)|^2 dr_2$$

$$- \psi_1^*(r)\psi_2(r) \int \psi_1^*(r_2)\psi_2(r_2)\, dr_2$$

$$- \psi_1(r)\psi_2^*(r) \int \psi_1(r_2)\psi_2^*(r_2)\, dr_2$$

Using $\int \psi_1^*(r)\,\psi_2(r)\, dr = 0$

Also, $\int \psi_1(r)\,\psi_2^*(r)\, dr = 0$

* Since $|\psi(r)|^2$ is radial probability density, its integral over r will be equal to 1

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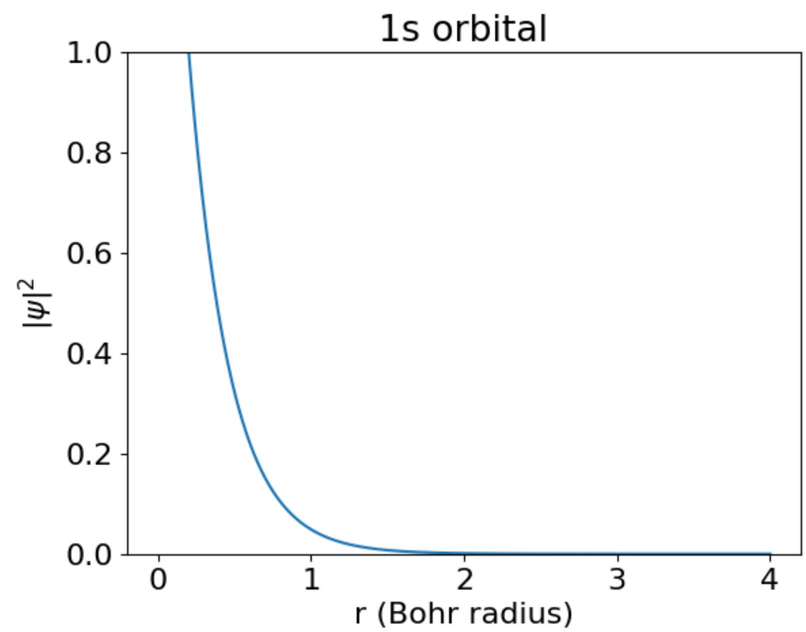
$$\Rightarrow \quad n(r) = |\psi_1(r)|^2 \times 1 + |\psi_2(r)|^2 \times 1 - 0 - 0$$

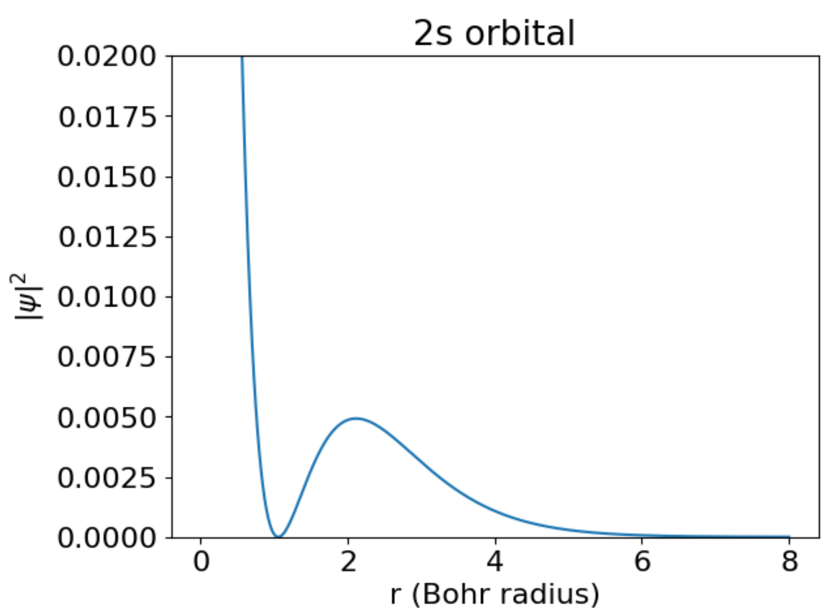
$$\Rightarrow \quad \boxed{n(r) = |\psi_1(r)|^2 + |\psi_2(r)|^2}$$

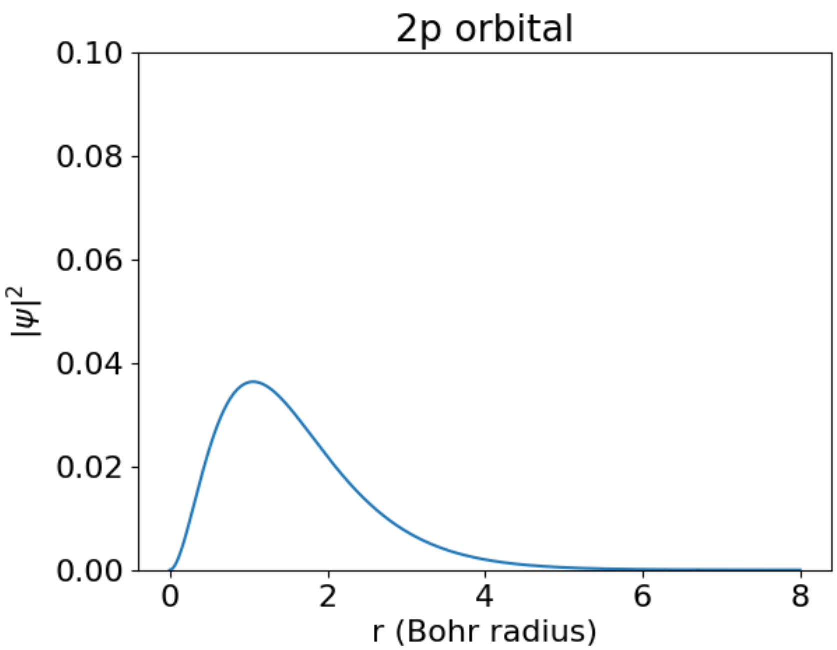
Q.2

Solution

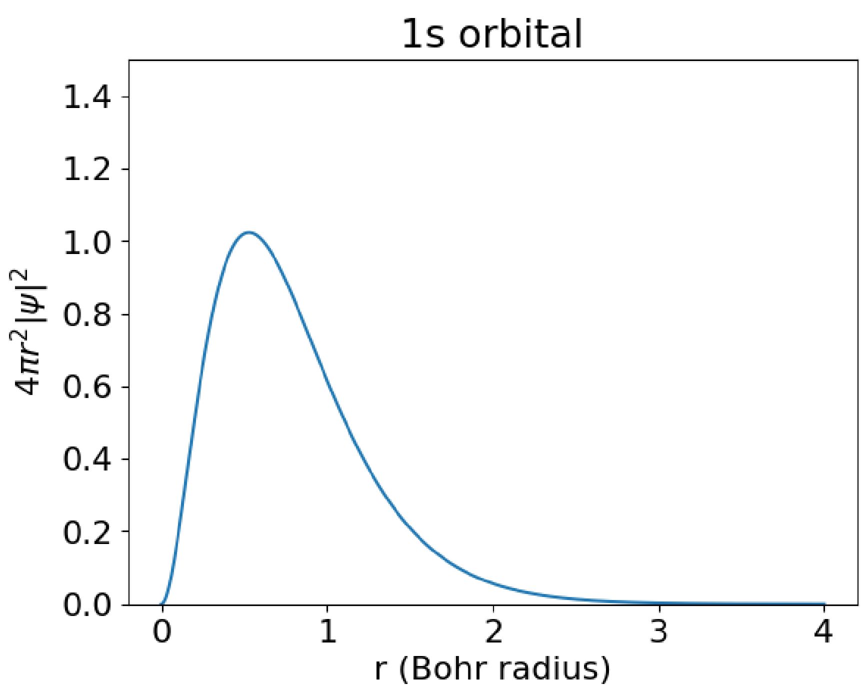
Plots for radial probability density $|\psi|^2 = \psi^* \psi$

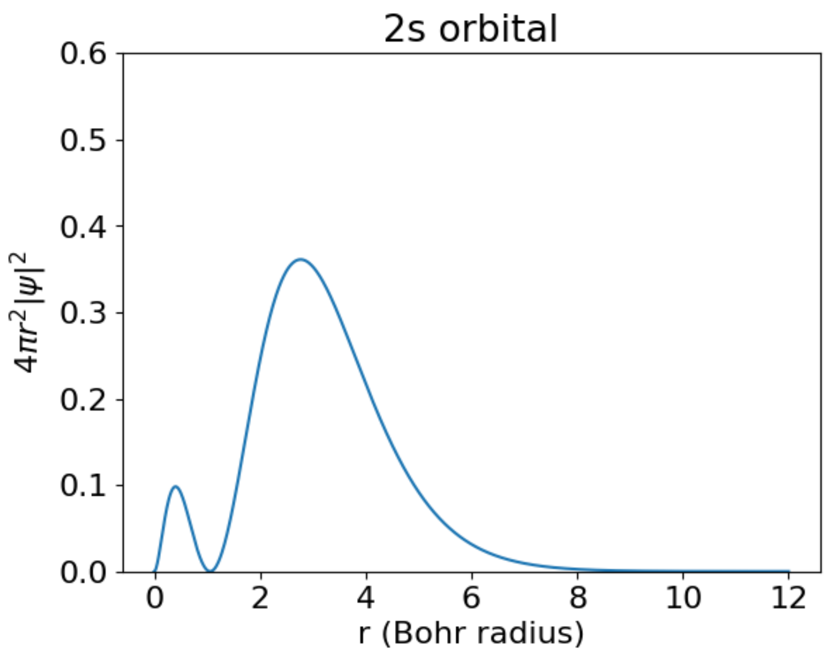


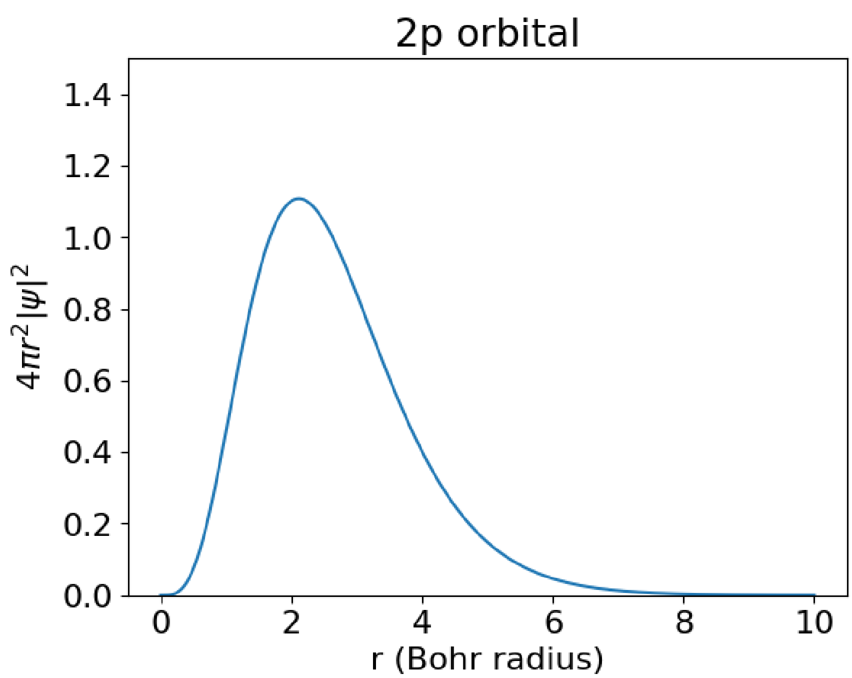




Plots for radial probability $4\pi r^2|\psi|^2$




2s orbital
0.6
0.5
0.4
0.3
0.2
0.1
0.0
$4\pi r^2|\psi|^2$
0
2
4
6
8
10
12
r (Bohr radius)


2p orbital
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
$4\pi r^2|\psi|^2$
0
2
4
6
8
10
r (Bohr radius)