

Homework I

Introduction to Physical Chemistry

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1 Question 1

$$\Phi_3 = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{3\pi x}{L}\right)$$

$$\begin{aligned}\Pr(0.15L \leq 0x \leq 0.17L) &= \int_{0.15L}^{0.17L} |\Phi_3(x)|^2 dx \\ &= \int_{0.15L}^{0.17L} \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{3\pi x}{L}\right) \cdot \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{3\pi x}{L}\right) dx \\ &= \frac{2}{L} \int_{0.15L}^{0.17L} \sin^2\left(\frac{3\pi x}{L}\right) dx\end{aligned}$$

$$\text{Let } u = \frac{3\pi x}{L}, \quad du = \frac{3\pi}{L} dx, \quad dx = \frac{L}{3\pi} du$$

$$\begin{aligned}\Pr(0.15L \leq 0x \leq 0.17L) &= \frac{2}{L} \int_{0.45\pi}^{0.51\pi} \frac{L}{3\pi} \sin^2(u) du \\ &= \frac{2}{3\pi} \int_{0.45\pi}^{0.51\pi} \frac{1}{2} (1 - \cos(2u)) du \\ &= \frac{1}{3\pi} \left[u - \frac{1}{2} \sin(2u) \right]_{0.45\pi}^{0.51\pi} \\ &= 0.1733 - 0.1336 \\ &= 0.0397\end{aligned}$$

2 Question 2

$$\begin{aligned} \text{total nodes} &= 5 \\ \text{total radial nodes} &= 5 \\ \text{(a) } \text{total nodes} &= n - 1 \\ n &= 5 \\ \text{total radial nodes} &= n - l - 1 \\ l &= 0 \end{aligned}$$

The associated orbital is 6s

$$\begin{aligned} \text{total nodes} &= 3 \\ \text{total radial nodes} &= 0 \\ \text{(b) } \text{total nodes} &= n - 1 \\ n &= 4 \\ \text{total radial nodes} &= n - l - 1 \\ l &= 3 \end{aligned}$$

The associated orbital is 4f

3 Question 3

(a) radial component: $\left[1 - \frac{1}{4} \left(\frac{r}{a_0}\right) + \frac{1}{80} \left(\frac{r}{a_0}\right)^2\right] \left(\frac{r}{a_0}\right)$

$$\left[1 - \frac{1}{4} \left(\frac{r}{a_0}\right) + \frac{1}{80} \left(\frac{r}{a_0}\right)^2\right] \left(\frac{r}{a_0}\right) = 0 \text{ where } r \neq 0$$

$$1 - \frac{1}{4} \left(\frac{r}{a_0}\right) + \frac{1}{80} \left(\frac{r}{a_0}\right)^2 = 0$$

$$r^2 - 20a_0r + 80a_0^2 = 0$$

$$(r - 10a_0)^2 - 100a_0^2 + 80a_0^2 = 0$$

$$(r - 10a_0)^2 = 20a_0^2$$

$$r = 10a_0 \pm \sqrt{20}a_0$$

Radial nodes exist when $r = (10 + \sqrt{20})a_0$ or $(10 - \sqrt{20})a_0$.

(b) There are two radial nodes

(c) angular component: $\sin \theta \sin \phi$
 $\sin \theta \sin \phi = 0$

(d) $4p_y$

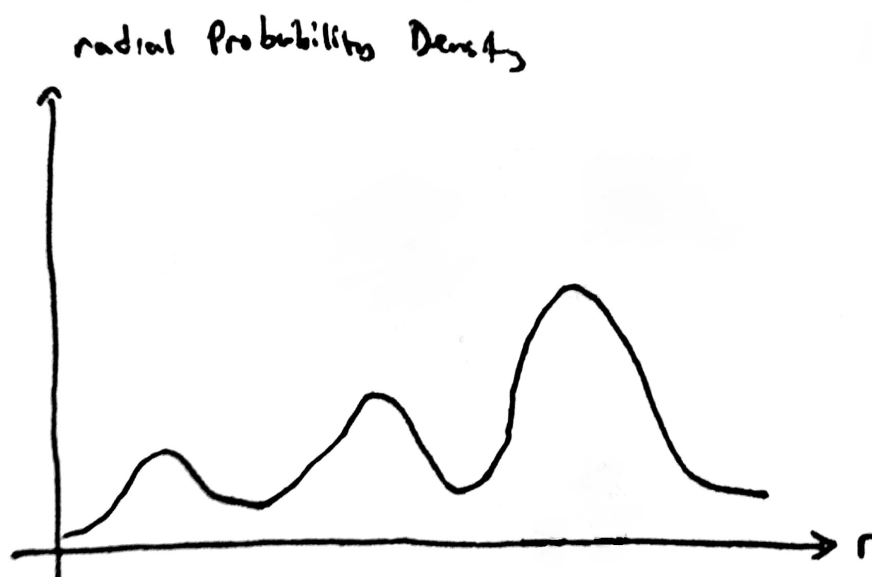


Figure 1: RPD Graph

(e)