❖ Probability Distribution Function

The probability distribution function is the behavior of ψ^2 at various points around the nucleus as a function of distance r from the nucleus. The plots of such functions are also called as the probability distribution curves. Nevertheless, since it is only the radial part ($R_{n,l}$) that varies with the distance from the nucleus, the graphs of ψ^2 must behave in the same manner. To understand this more precisely, consider the plot of the first two quantum mechanical states of an electron in a hydrogen atom.

➢ *Probability Distribution of $\psi_{1,0,0}$ State (1s Orbital)*

In order to understand the probability distribution function of the electron in the ground state of the hydrogen atom, recall the mathematical expression for the same i.e.

$$\psi_{1,0,0} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} \tag{429}$$

Squaring both sides, we get

$$\psi_{1,0,0}^2 = \frac{1}{\pi a_0^3} e^{-2r/a_0} \tag{430}$$

It is obvious from the equation (429, 430) that the pre-exponential part is simply a constant and variation depends only upon the exponential part.

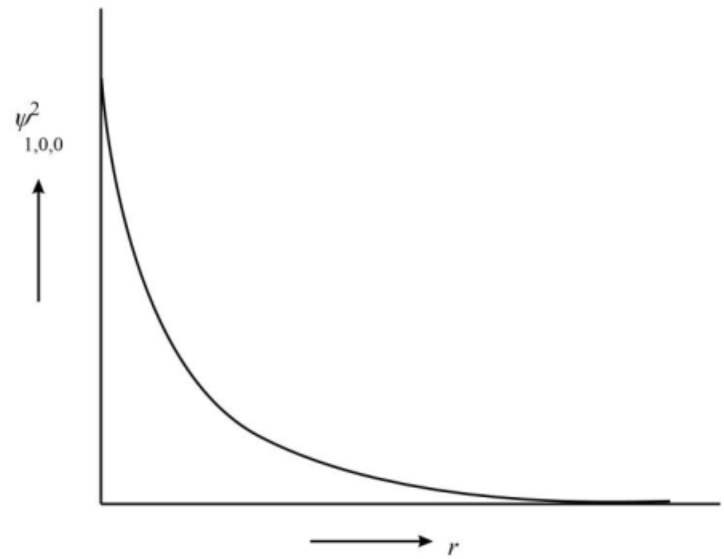

Figure 21. The variation of electron density vs distance from the center of the nucleus in 1*s* orbital.

Hence, it can be concluded that the density of the electron wave is highest at the center of the nucleus and decreases as the distance from the center of the nucleus increases, and becomes zero only at infinite.

➢ ***Probability Distribution of $\psi_{2,0,0}$ State (2s Orbital)***

In order to understand the probability distribution function of an electron in the 2*s* state of the hydrogen atom, recall the mathematical expression for the same i.e.

$$\psi_{2,0,0} = \frac{1}{4\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0} \tag{431}$$

Squaring both sides, we get

$$\psi_{2,0,0}^2 = \frac{1}{16\pi a_0^3}\left(2 - \frac{r}{a_0}\right)^2 e^{-r/a_0} \tag{432}$$

It is obvious from the equation (431, 432) that the pre-exponential part is simply a constant and variation depends only upon the exponential part.

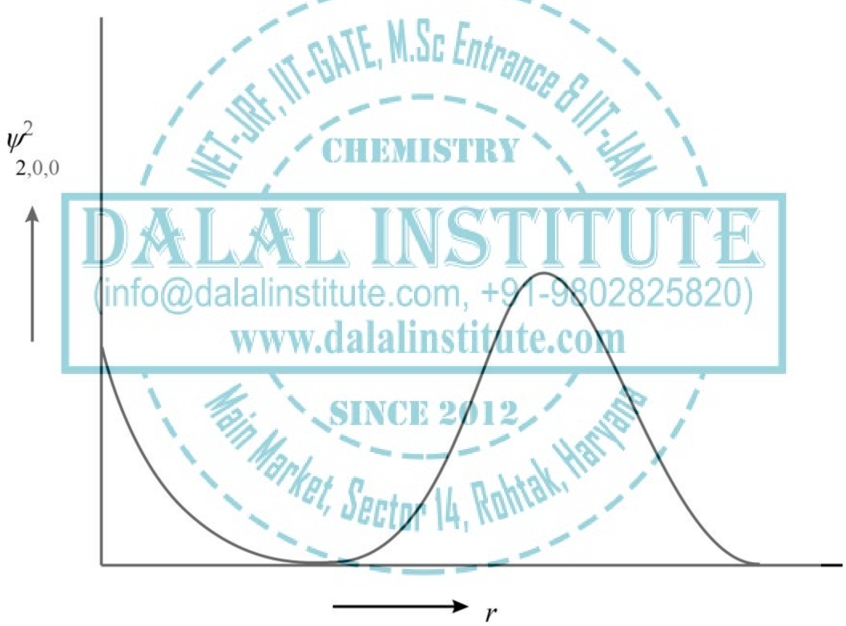

Figure 22. The variation of electron density vs distance from the center of the nucleus in 2*s* orbital.

Hence, it can be concluded that the density of electron wave is non zero at the center of the nucleus and decreases as the distance from the center of the nucleus increases, and becomes zero at $r = 2a_0$. Now since the wave function changes sign after $2a_0$, the density of electron wave after that increases first and then decreases exponentially and finally becomes zero at infinite distance. Now it's quite confusing because we have been told that the electron cannot reside within the nucleus and the probability of finding the electron inside the nucleus is almost zero, meaning that there must be something else that also governs the probability.

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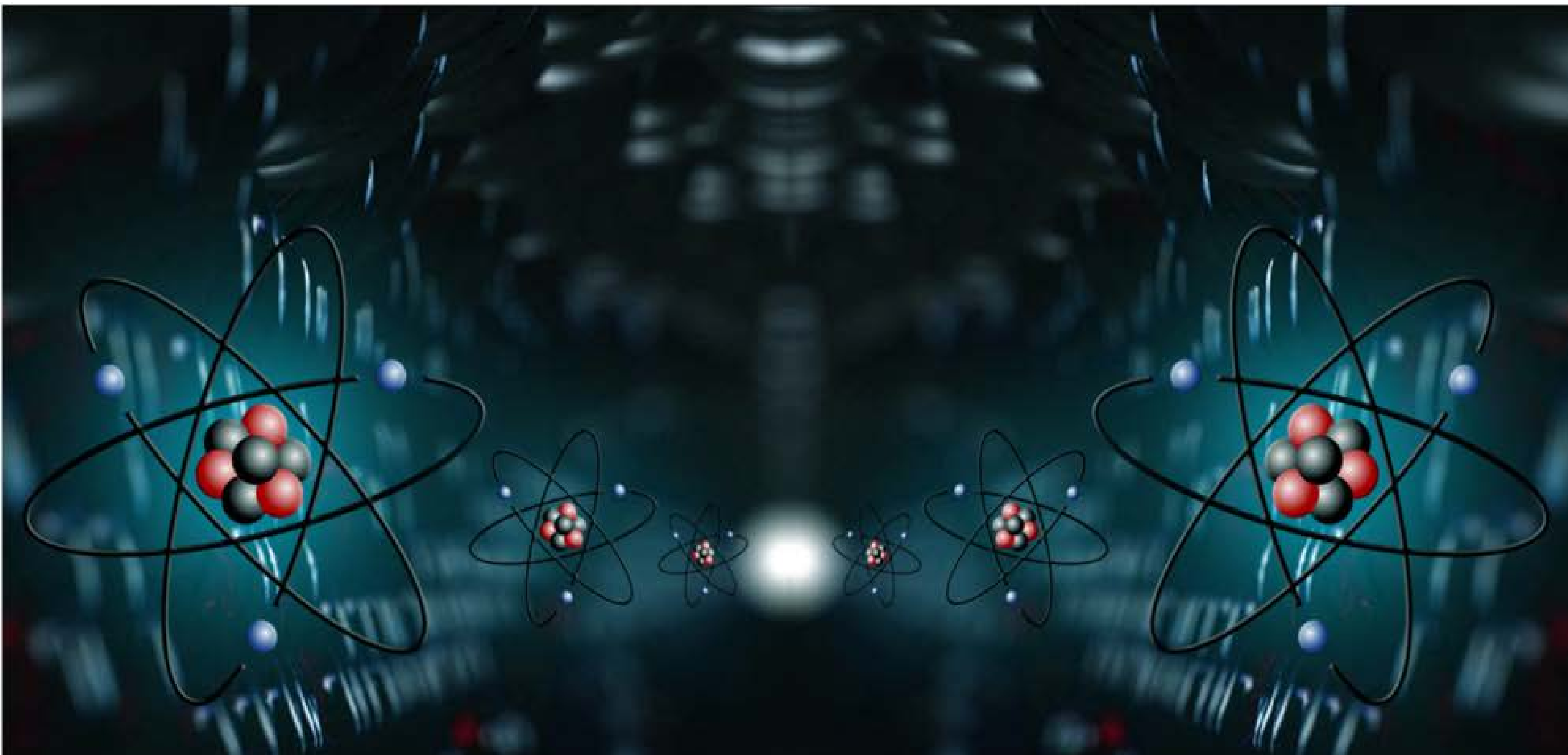

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