CH107: Week 4

Arihant Vashista, 22B0958

11^{th} January 2023

1 Wave-function for n = 2

In the last week's assignment we covered s orbital wave functions. Next we plotted the radial wave functions for p orbitals for n = 2.Here $\Psi_{2,1,0}$ is a real valued function but the $\Psi_{2,1,\pm1}$ are not real valued because of the $e^{\pm i\phi}$ term. Hence we perform Linear combination of the $m = \pm 1$ functions to get real valued ψ_{2p_x} and ψ_{2p_y} in terms of θ and ϕ. This is the plot of radial functions of of 2p orbital. $R(r)^2 vs\, r$.

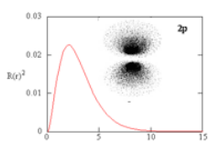

Figure 1: fig 1

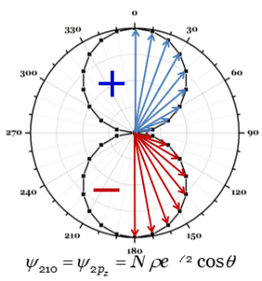

Figure 2: fig 2

We then studied the polar plot of the of the angular part of the $2p_z$ orbital, which is equal to $cos\theta$. It is represented as the second figure above.

2 Graphical Interpretation of Atomic Orbitals

Note that the angular wave functions dont have an actual physical meaning. Their plot cannot be regared as the "picture" of atomic orbital. Note that the **definition** of an **orbital** is an 1-electron wavefunction.

To represent the orbitals on graphs we plotted the **contour representation** of the wave functions . For that we first plotted the surface plots of ψ^2 and then represented their contour plots .We also learned how to find the **number of radial and angular nodes** using the wave function and its graphical plot. Also note that in the **contour plots** the **radial nodes** are represented as **circles** and the **angular nodes** are represented as **straight lines** Following are examples of a few contour plots:-

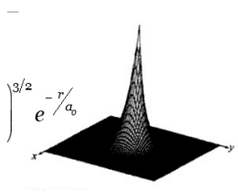

Figure 3: Surface Plot

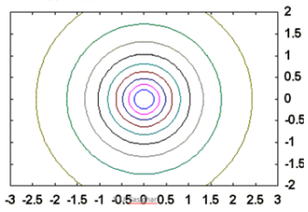

Figure 4: Contour Plot

Figure 5: **1s orbital**

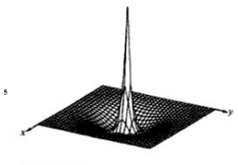

Figure 6: Surface Plot

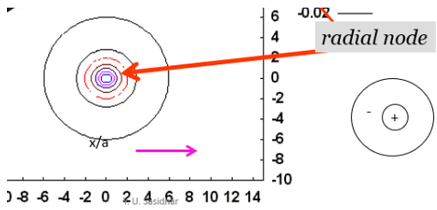

Figure 7: Contour Plot

Figure 8: **2s orbital**

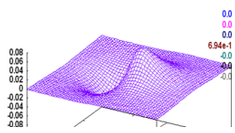

Figure 9: Surface Plot

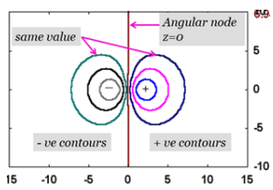

Figure 10: Contour Plot

Figure 11: **$2p_z$ orbital**

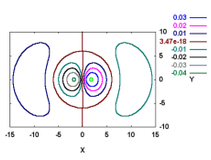

Figure 12: 3pz

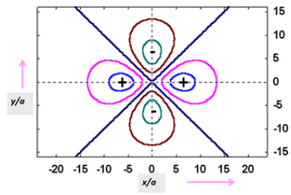

Figure 13: $3dx^2 - y^2$

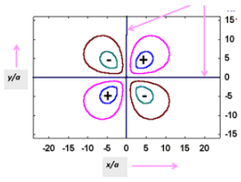

Figure 14: $3d_{xy}$

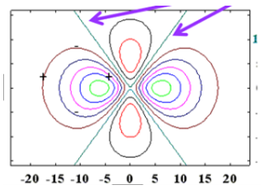

Figure 15: $3dz^2$

3 Conclusion

Summary of all the wave functions of hydrogen atom.Apllication of these are sued to explain the **excited states , atomic spectra and other many electron atoms**.