

Blog Entry © Sunday, November 9, 2025, by James Pate Williams, Jr. Hydrogenic Wavefunctions, Radial Probability Functions, Distribution Functions, and First Moment Integrals

References:

<http://www.hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydwf.html#c3>

<https://dasher.wustl.edu/chem478/reading/frontier-orbitals-anh.pdf>

**The Nature of the Chemical Bond** © 1960 by Linus Pauling

**Quantum Mechanics Third Edition** © 1968 by Leonard I. Schiff

$$\langle r \rangle = \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} r^3 \sin \vartheta \psi_{nlm}^*(r, \vartheta, \varphi) \psi_{nlm}(r, \vartheta, \varphi) dr d\vartheta d\varphi$$

| #  | Z | n | l | m  | <r>    | <r>  | % Error  |
|----|---|---|---|----|--------|------|----------|
| 1  | 1 | 1 | 0 | 0  | 1.498  | 1.5  | 0.1541   |
| 2  | 1 | 2 | 0 | 0  | 5.996  | 6    | 0.05867  |
| 3  | 1 | 2 | 1 | 1  | 4.998  | 5    | 0.03486  |
| 4  | 1 | 2 | 1 | 0  | 5.002  | 5    | 0.04295  |
| 5  | 1 | 2 | 1 | -1 | 4.998  | 5    | 0.03467  |
| 6  | 1 | 3 | 0 | 0  | 13.5   | 13.5 | 0.01051  |
| 7  | 1 | 3 | 1 | 1  | 12.5   | 12.5 | 0.007391 |
| 8  | 1 | 3 | 1 | 0  | 12.5   | 12.5 | 0.02153  |
| 9  | 1 | 3 | 1 | -1 | 12.51  | 12.5 | 0.07035  |
| 10 | 1 | 3 | 2 | 2  | 10.5   | 10.5 | 0.02792  |
| 11 | 1 | 3 | 2 | 1  | 10.5   | 10.5 | 0.008593 |
| 12 | 1 | 3 | 2 | 0  | 10.49  | 10.5 | 0.0612   |
| 13 | 1 | 3 | 2 | -1 | 10.48  | 10.5 | 0.1447   |
| 14 | 1 | 3 | 2 | -2 | 10.5   | 10.5 | 0.01272  |
| 15 | 2 | 1 | 0 | 0  | 0.7498 | 0.75 | 0.02608  |
| 16 | 2 | 2 | 0 | 0  | 3.004  | 3    | 0.1221   |
| 17 | 2 | 2 | 1 | 1  | 2.501  | 2.5  | 0.04773  |
| 18 | 2 | 2 | 1 | 0  | 2.5    | 2.5  | 0.01789  |
| 19 | 2 | 2 | 1 | -1 | 2.503  | 2.5  | 0.1232   |
| 20 | 2 | 3 | 0 | 0  | 6.749  | 6.75 | 0.00992  |
| 21 | 2 | 3 | 1 | 1  | 6.245  | 6.25 | 0.08021  |
| 22 | 2 | 3 | 1 | 0  | 6.252  | 6.25 | 0.02939  |
| 23 | 2 | 3 | 1 | -1 | 6.245  | 6.25 | 0.07904  |
| 24 | 2 | 3 | 2 | 2  | 5.252  | 5.25 | 0.0344   |
| 25 | 2 | 3 | 2 | 1  | 5.249  | 5.25 | 0.02673  |
| 26 | 2 | 3 | 2 | 0  | 5.249  | 5.25 | 0.009635 |
| 27 | 2 | 3 | 2 | -1 | 5.241  | 5.25 | 0.1784   |
| 28 | 2 | 3 | 2 | -2 | 5.251  | 5.25 | 0.009679 |

Table 1 Experimental <r> and Theory <r>

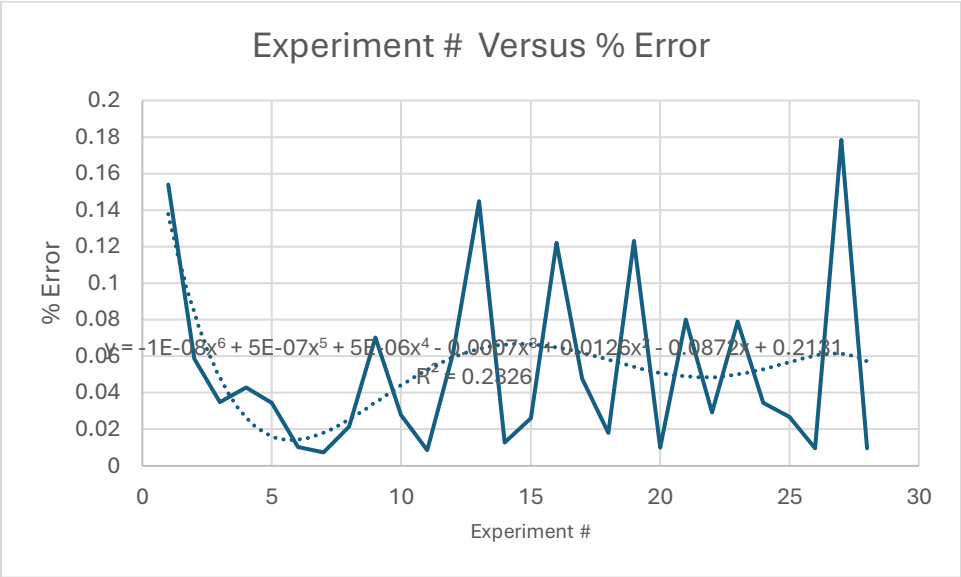


Figure 1 - Experiment  $\langle r \rangle$  Versus Percent Error

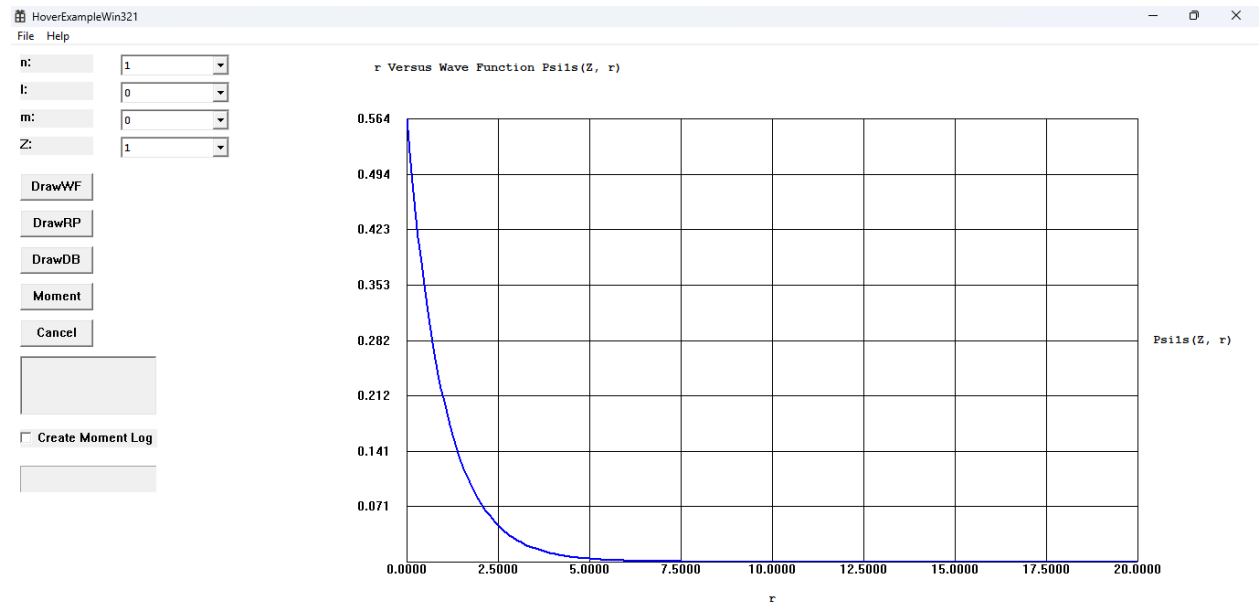


Figure 2 - r Versus Wavefunction  $1s\ 1, 0, 0, 1$

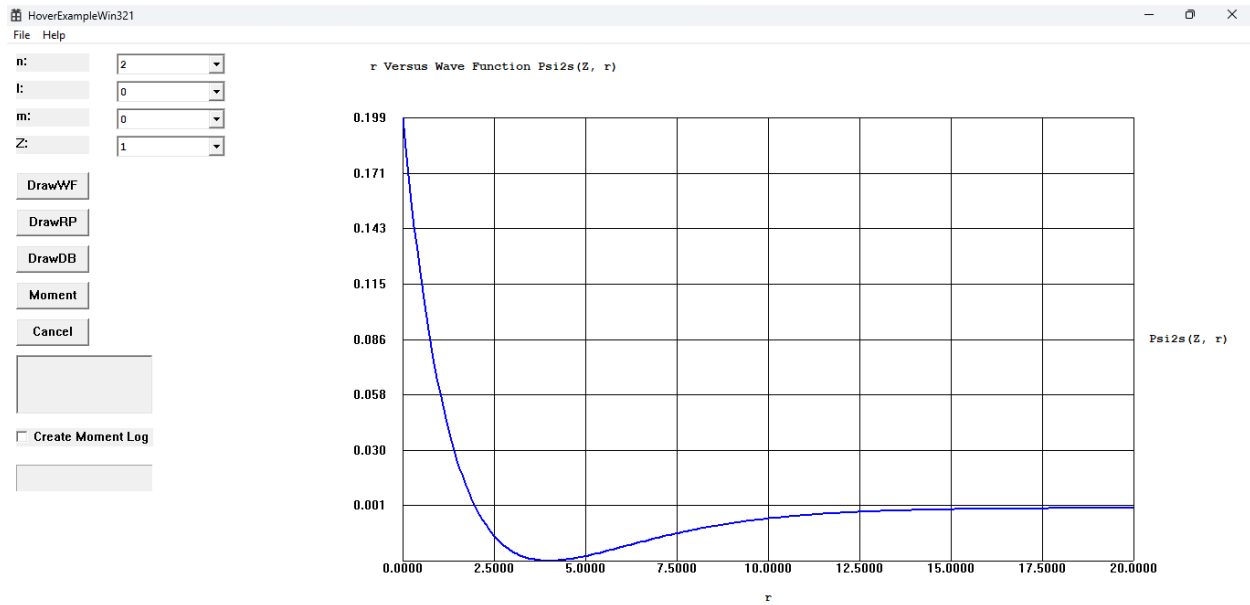


Figure 3 -  $r$  Versus Wavefunction  $2s\ 2,0,0,1$

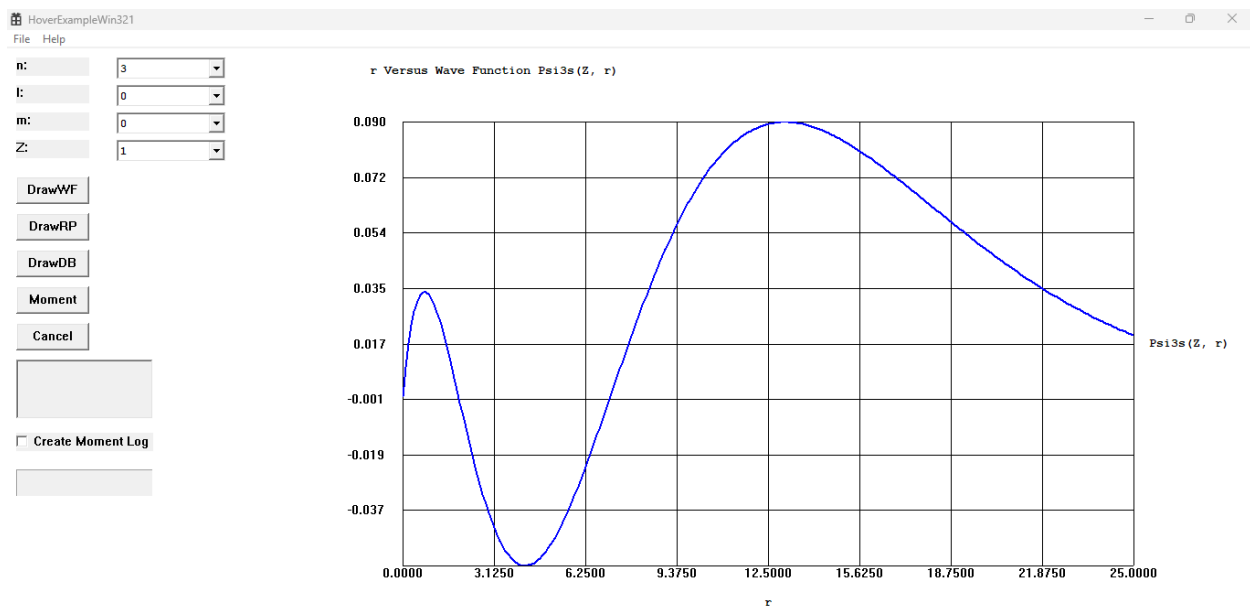


Figure 4 -  $r$  Versus  $3s\ 3,0,0,1$

$$RBF = 4\pi r^2 R_{nl}^2(r) \sin \vartheta$$

We use the Monte Carlo integration technique to compute the radial distribution function, RBF. See references above.

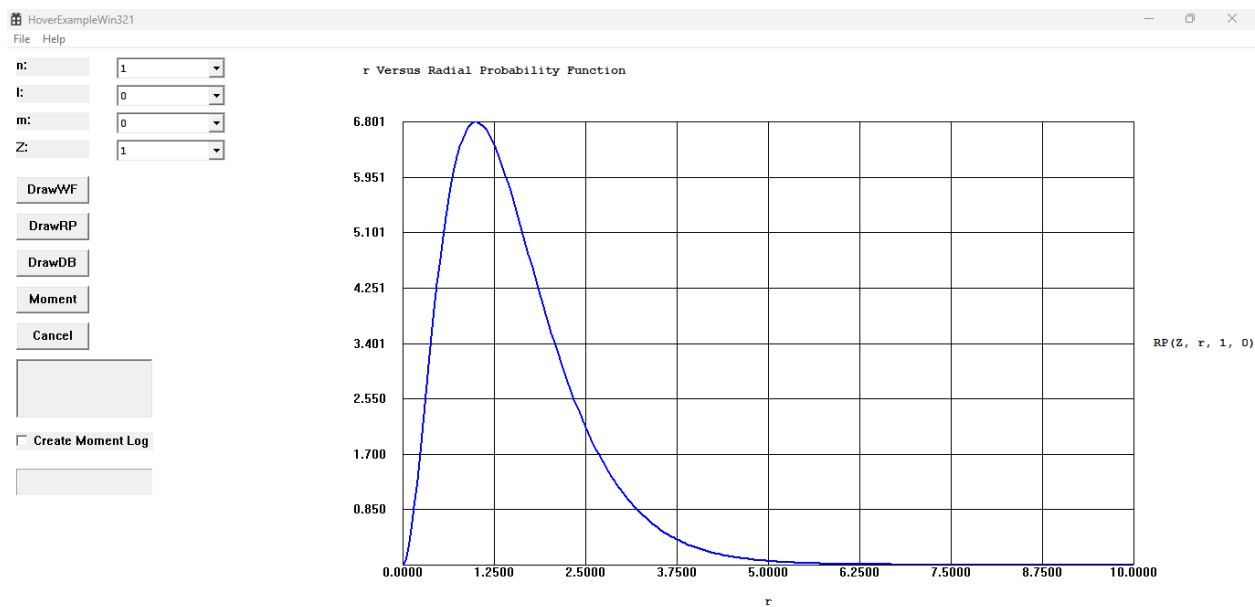


Figure 5 - Radial Probability Function for the 1s Orbital

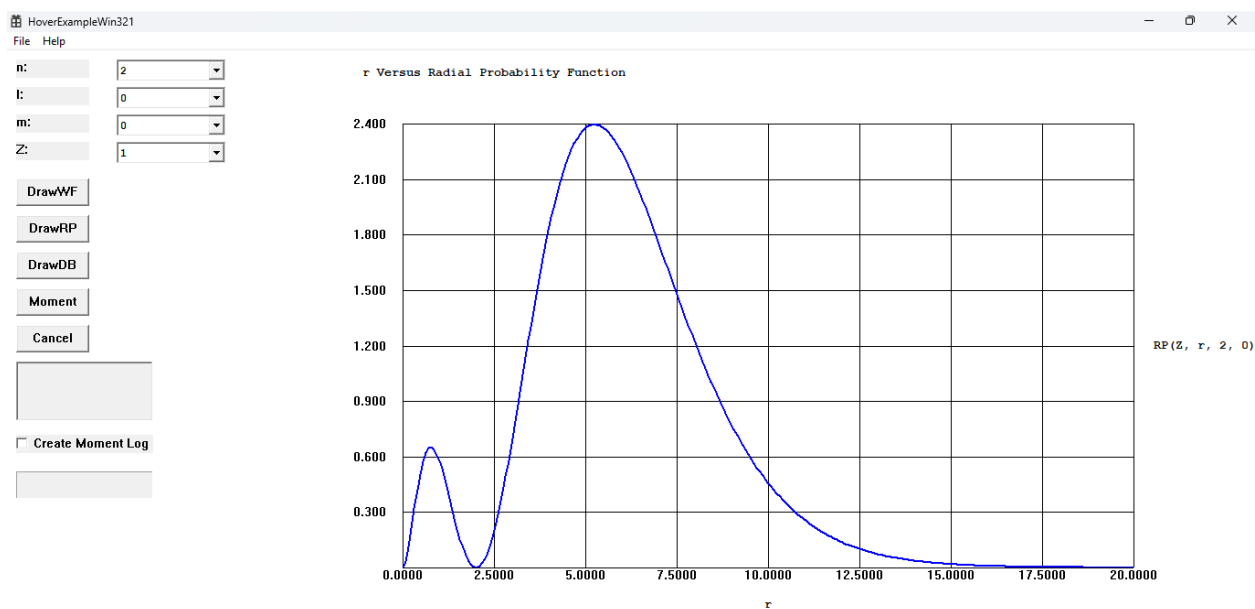


Figure 6 - Radial Probability Function for the 2s Orbital

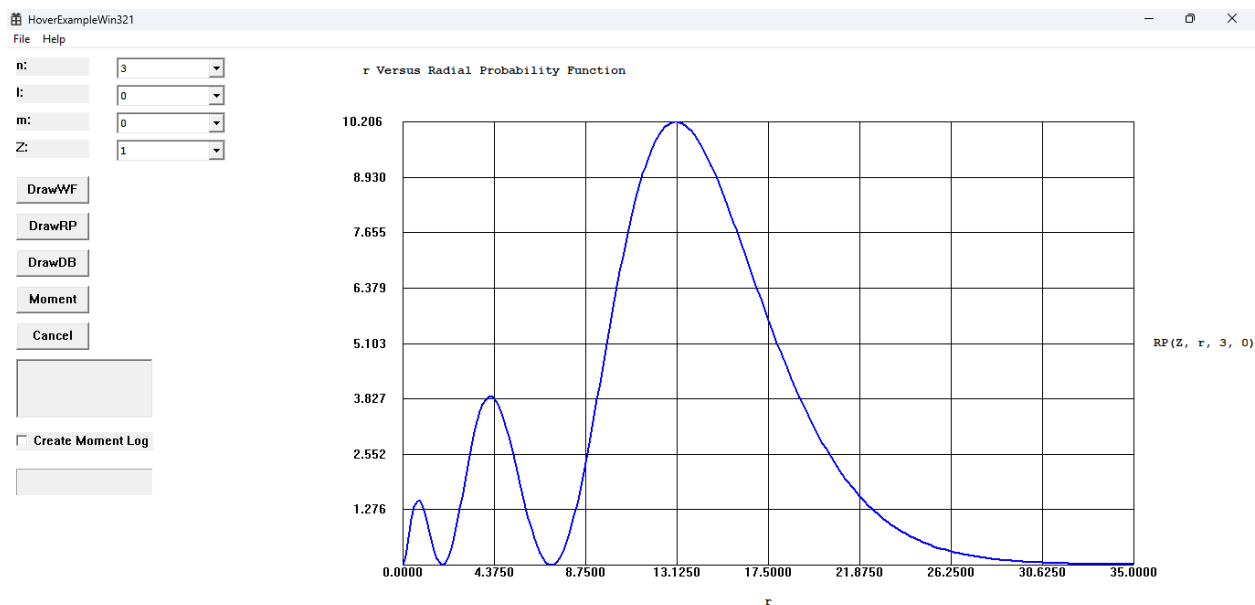


Figure 7 - Radial Probability Function for the 3s Orbital

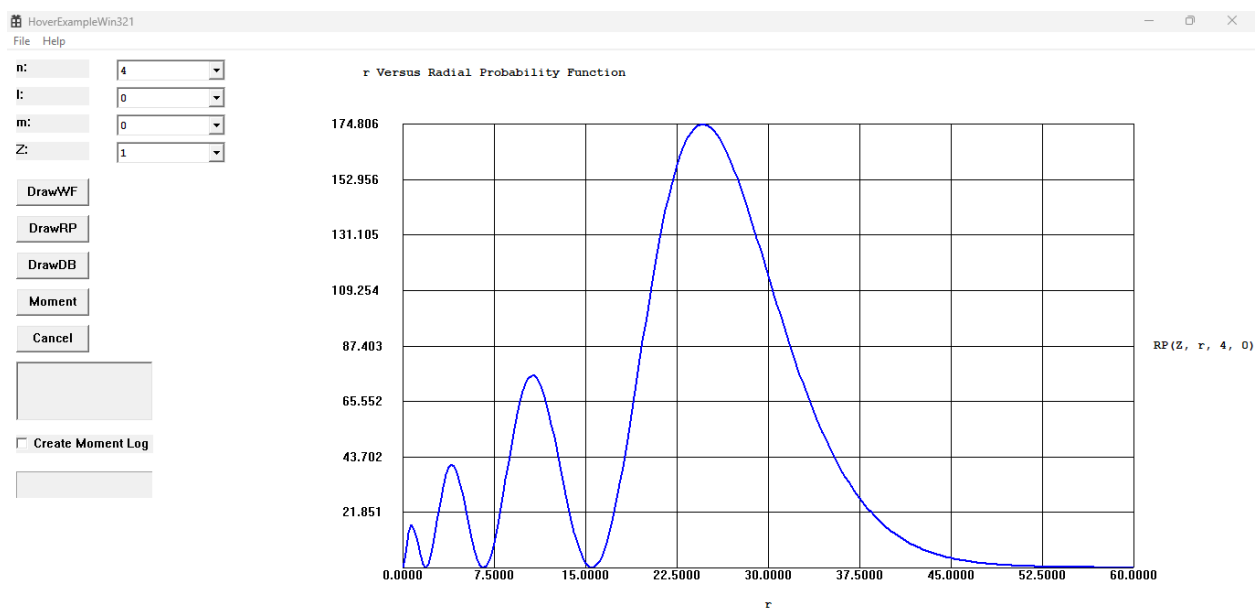


Figure 8 Radial Probability Function for the 4s Orbital

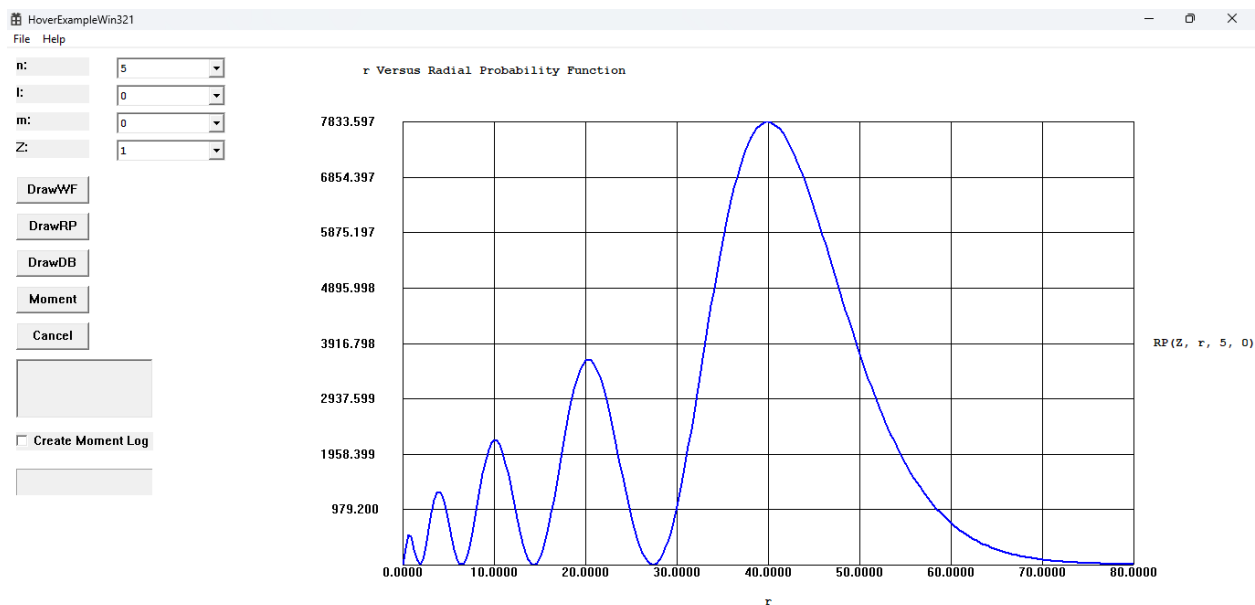


Figure 9 - Radial Probability Function for the 5s Orbital

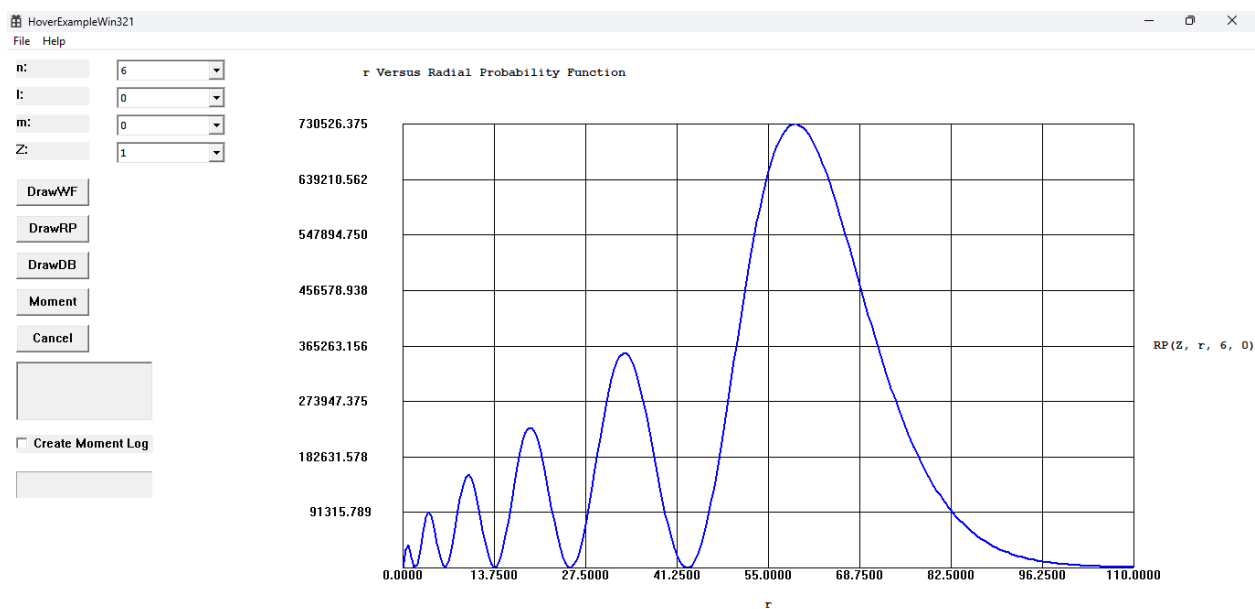


Figure 10 - Radial Probability Function for the 6s Orbital

HoverExampleWin321

File Help

n: 1

l: 0

m: 0

Z: 1

DrawWF

DrawRP

DrawDB

Moment

Cancel

<r> = 1.497688  
<r> = 1.500000

☐ Create Moment Log

Figure 11 - Single Moment Calculation

|                                                                 |   |
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