

Hydrogen-like Atomic Radial Wave Functions, Radial Probability Distribution Functions, Radial Probability Spherical Shell Distribution Functions by James Pate Williams, Jr. and Microsoft's Copilot

The hydrogen-like atom's radial wave function consists of an associated Laguerre polynomial and an exponential function [1] [2] [3] [4] [5]:

$$R_{nl}(r) = - \left\{ \left(\frac{2Z}{na_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho)$$

$$a_0 = \frac{\hbar^2}{\mu e^2}$$

$$\rho = \frac{2Z}{na_0} r, a_0 = 1 \text{ in this work, i. e. we use atomic units}$$

The Radial Electron Probability Distribution function is:

$$P(r) = r^2 |R_{nl}(r)|^2$$

The Radial Electron Probability Distribution Shell function is:

$$P_{shell}(r) = 4\pi r^2 |R_{nl}(r)|^2$$

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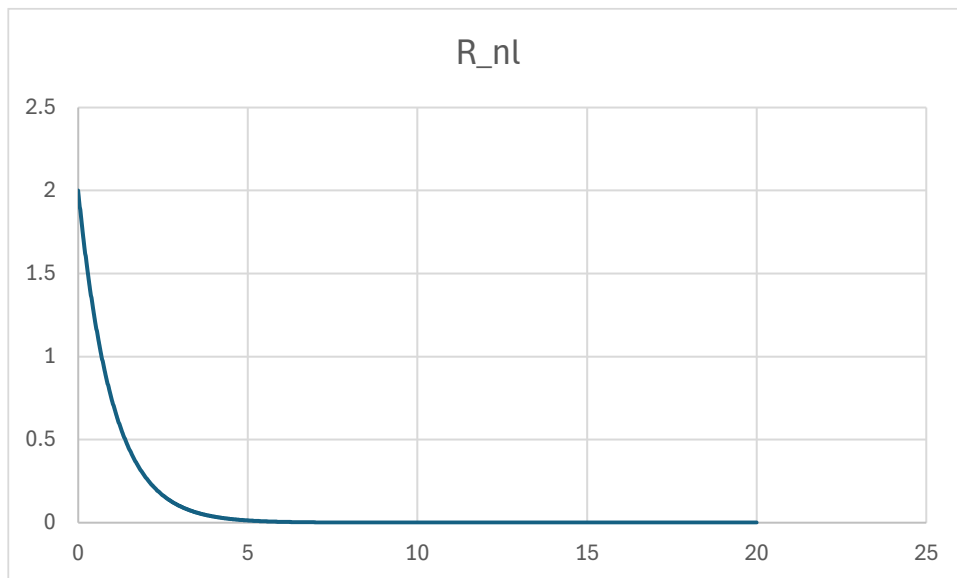


Figure 1 $R_{nl}(r)$ for $Z = 1, n = 1, l = 0, a_0 = 1$

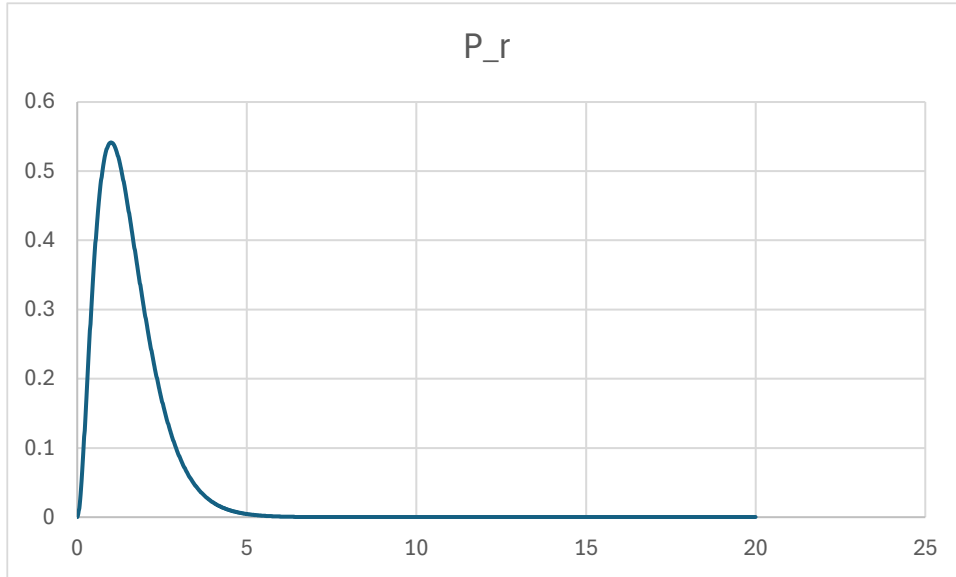


Figure 2 Radial Electron Probability Distribution Function for $Z = 1, n = 1, l = 0, a_0 = 1$

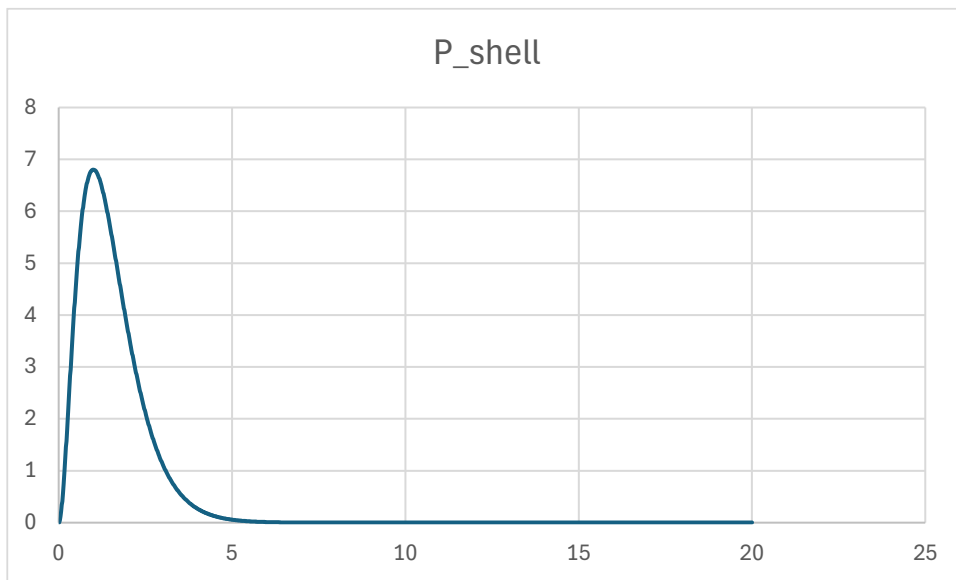


Figure 3 Radial Electron Probability Distribution Shell Function for $Z = 1, n = 1, l = 0, a_0 = 1$

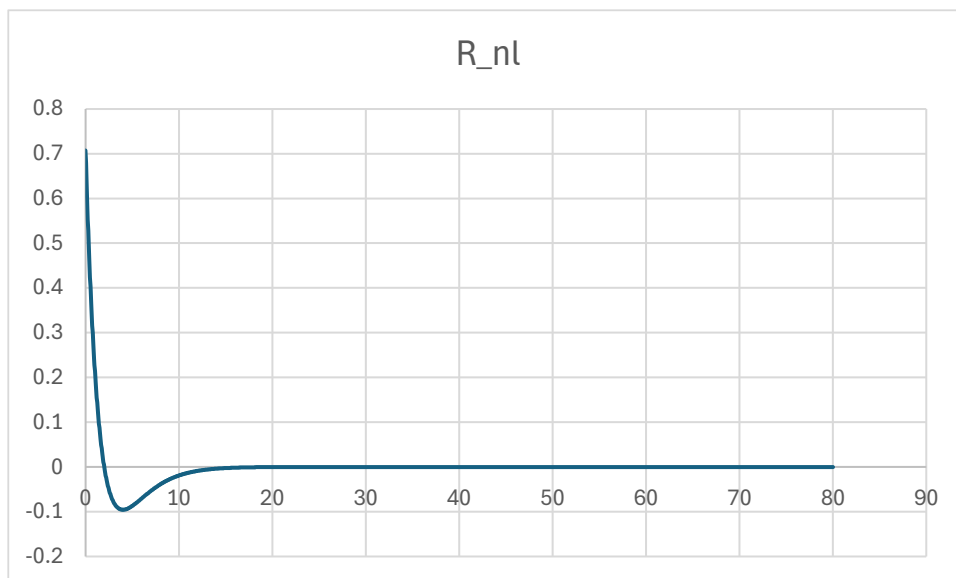


Figure 4 $R_{nl}(r)$ for $Z = 1$, $n = 2$, $l = 0$, $a_0 = 1$

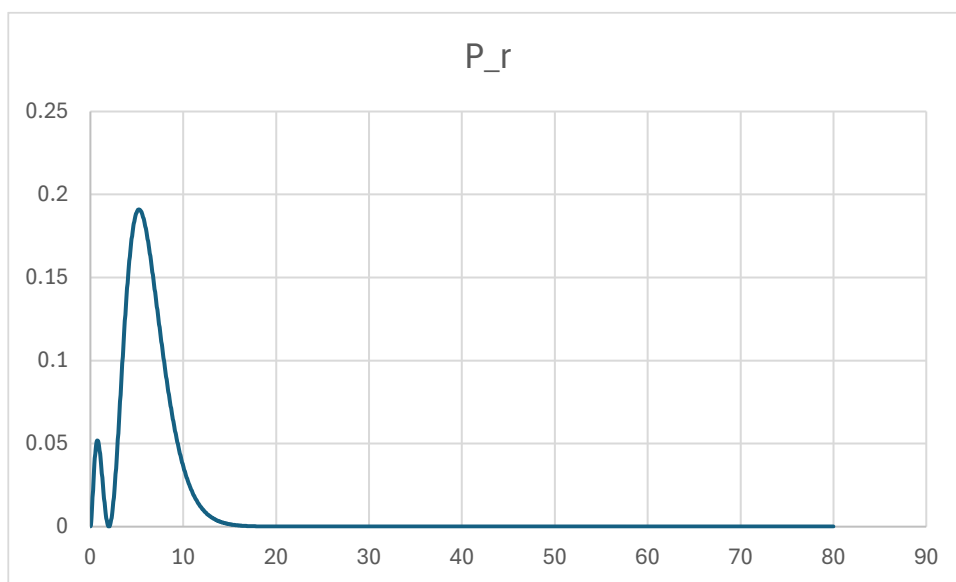


Figure 5 Radial Electron Probability Distribution Function for $Z = 1$, $n = 2$, $l = 0$, $a_0 = 1$

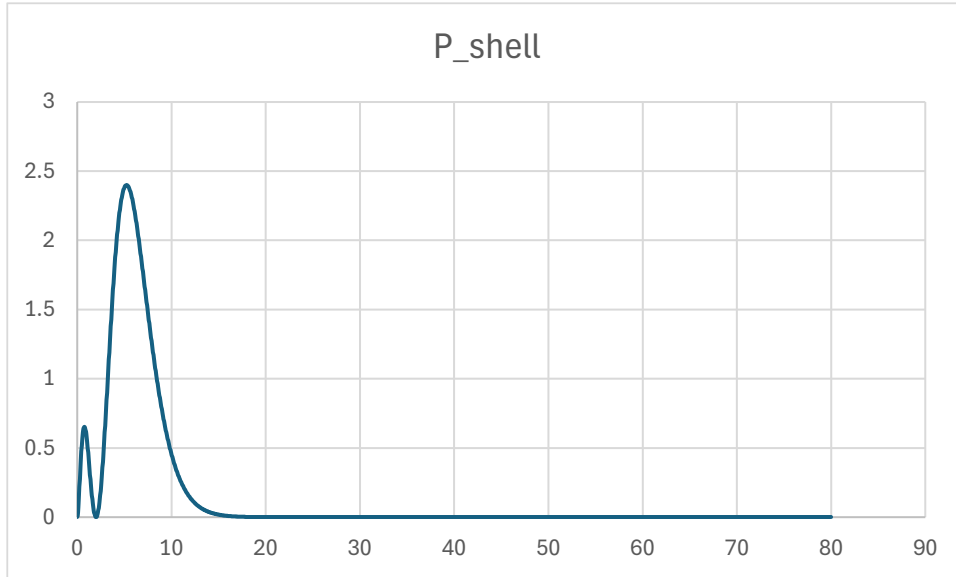


Figure 6 Radial Electron Probability Distribution Shell Function for $Z = 1, n = 2, l = 0, a_0 = 1$

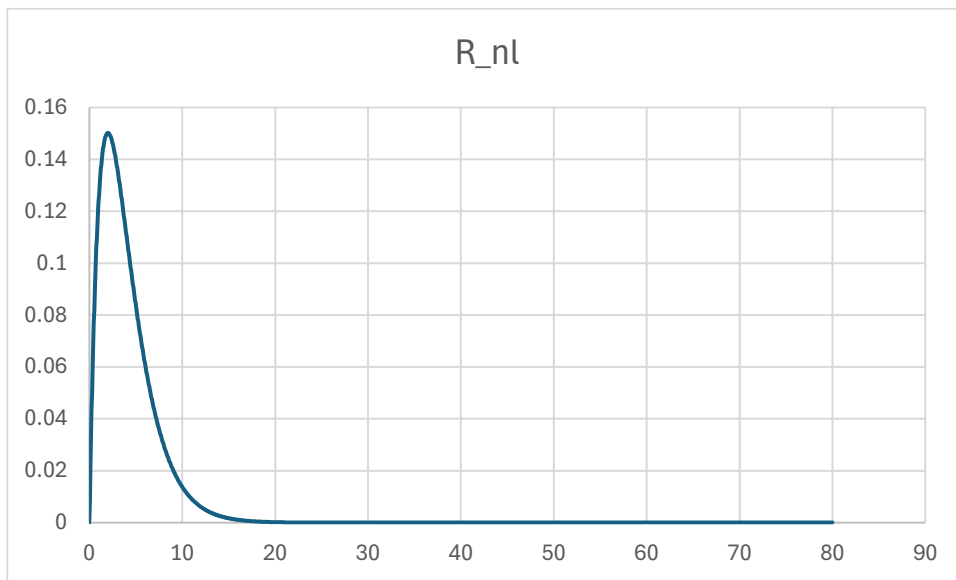


Figure 7 $R_{nl}(r)$ for $Z = 1, n = 2, l = 1, a_0 = 1$

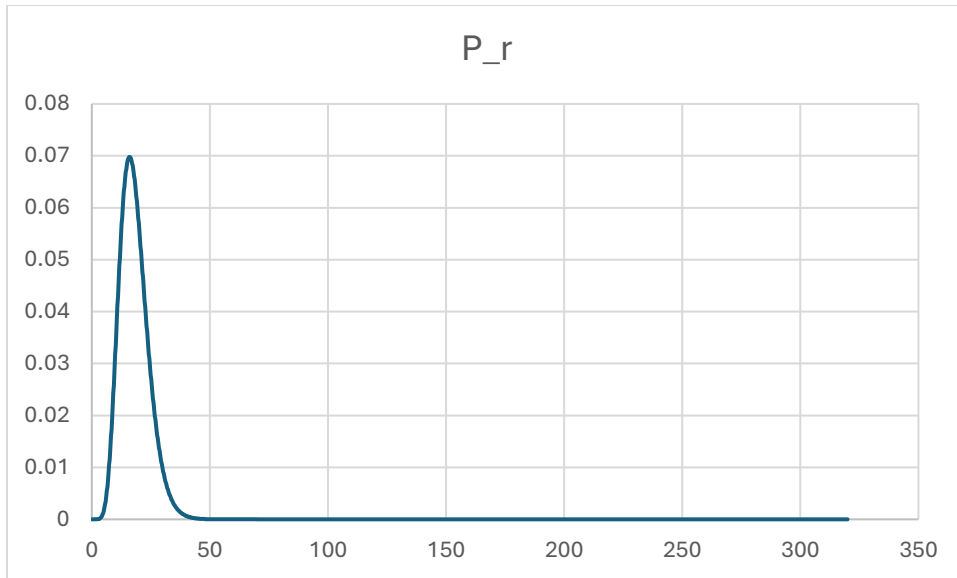


Figure 8 Radial Electron Probability Distribution Function for $Z = 1, n = 2, l = 0, a_0 = 1$

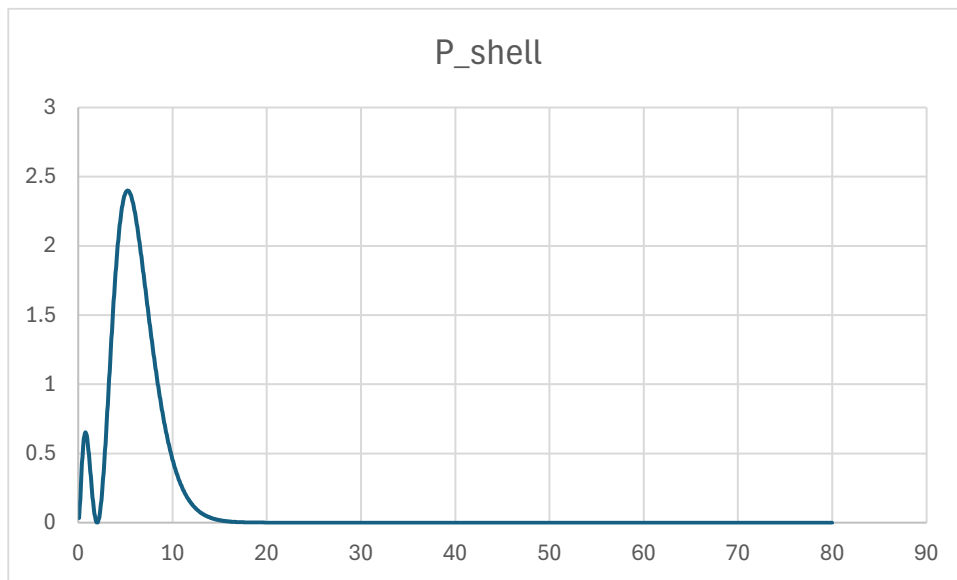


Figure 9 Radial Electron Probability Distribution Shell Function for $Z = 1, n = 2, l = 0, a_0 = 1$

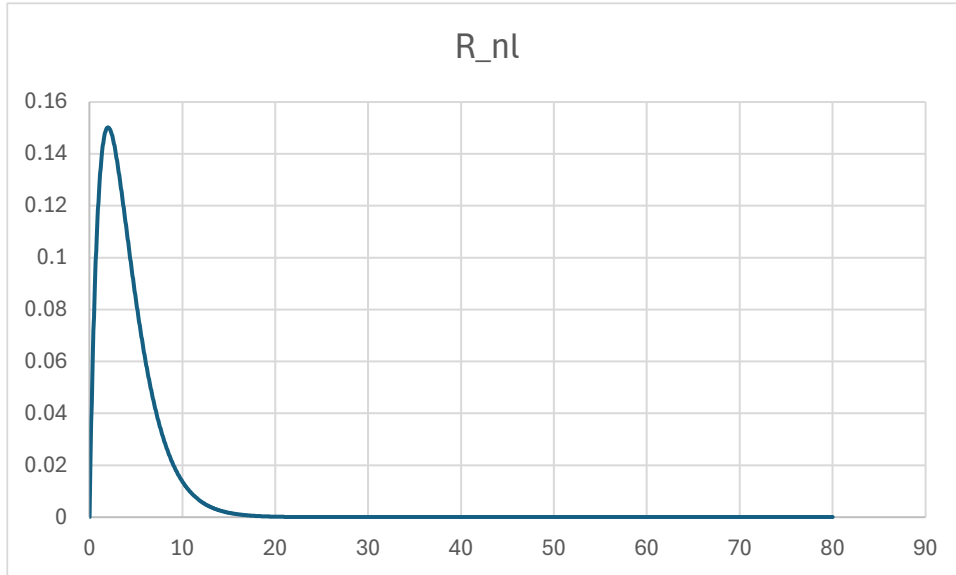


Figure 10 $R_{nl}(r)$ for $Z = 1$, $n = 2$, $l = 1$, $a_0 = 1$

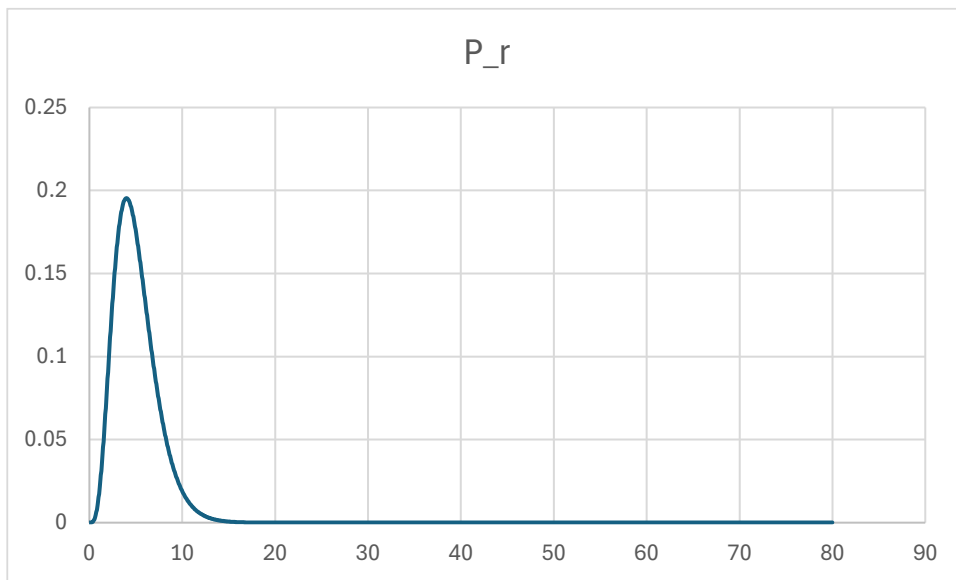


Figure 11 Radial Electron Probability Distribution Function for $Z = 1$, $n = 2$, $l = 1$, $a_0 = 1$

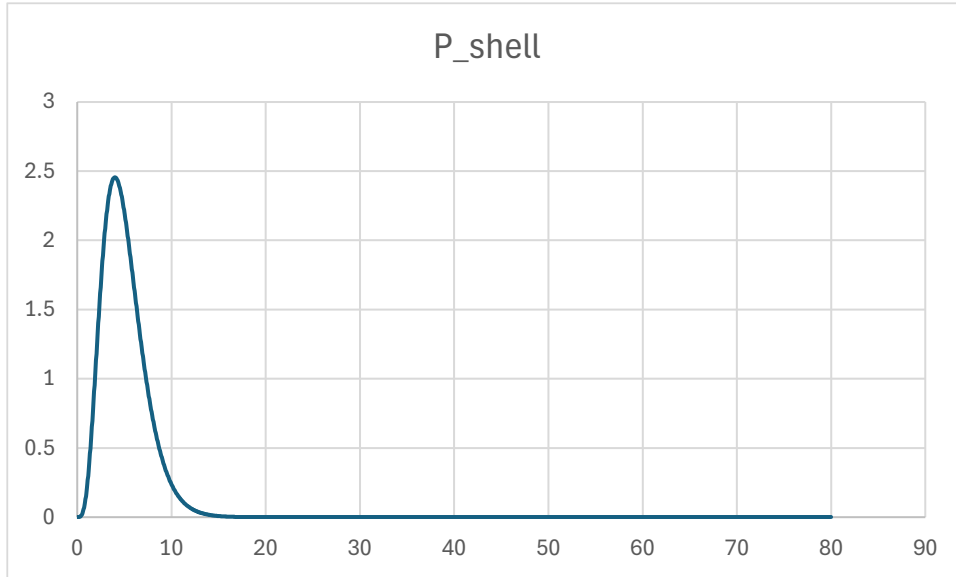


Figure 12 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 2$, $l = 1$, $a_0 = 1$

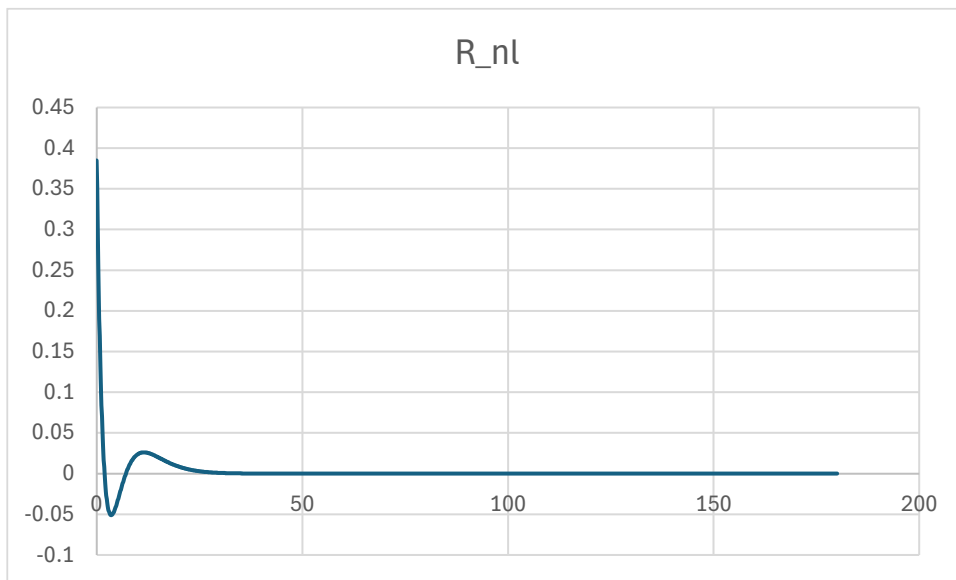


Figure 13 $R_{nl}(r)$ for $Z = 1$, $n = 3$, $l = 0$, $a_0 = 1$

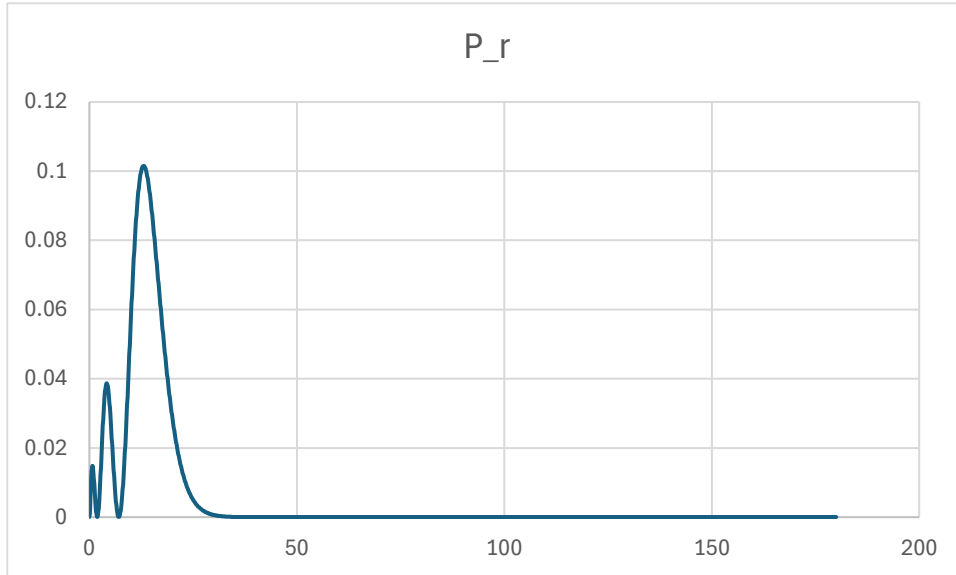


Figure 14 Radial Electron Probability Distribution Function for $Z = 1$, $n = 3$, $l = 0$, $a_0 = 1$

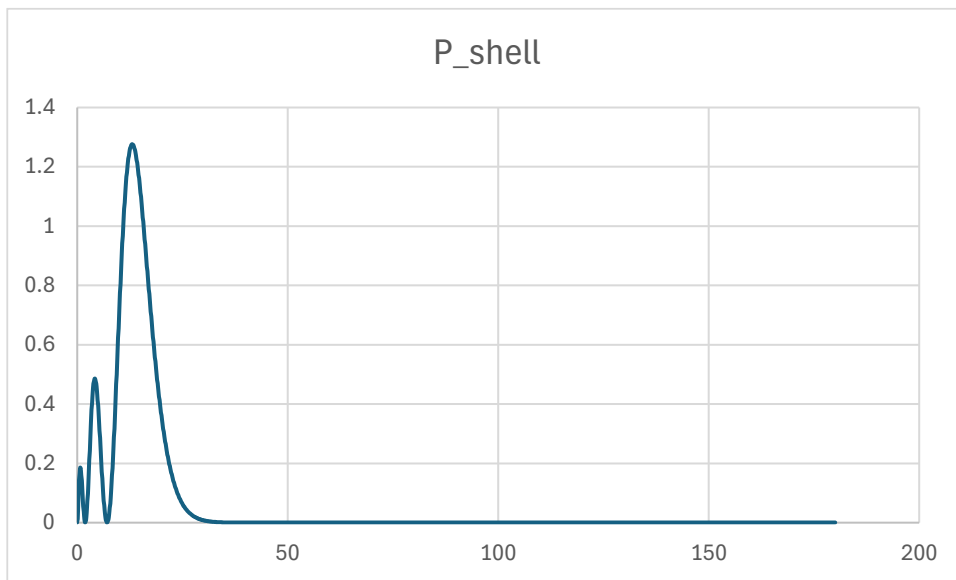


Figure 15 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 3$, $l = 0$, $a_0 = 1$

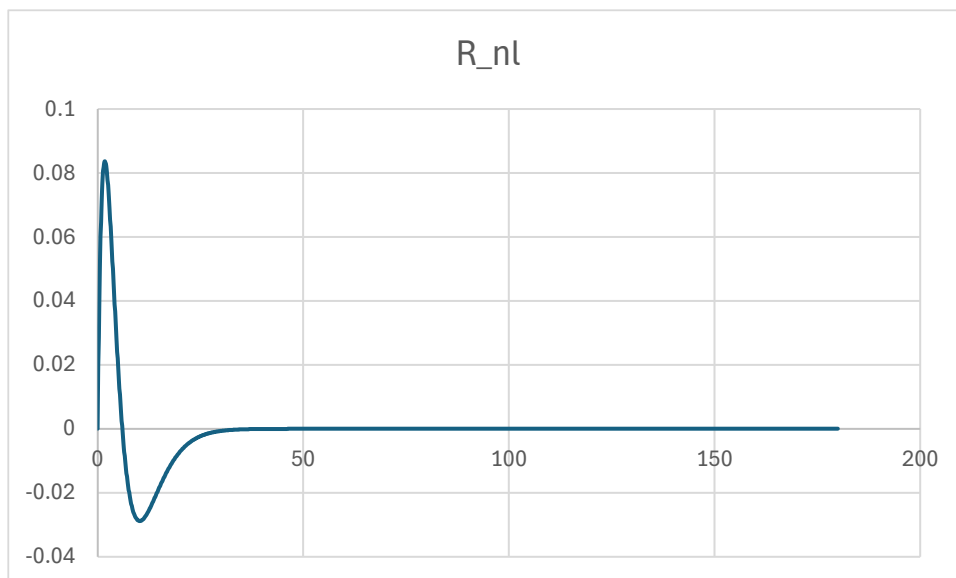


Figure 16 $R_{nl}(r)$ for $Z = 1, n = 3, l = 1, a_0 = 1$

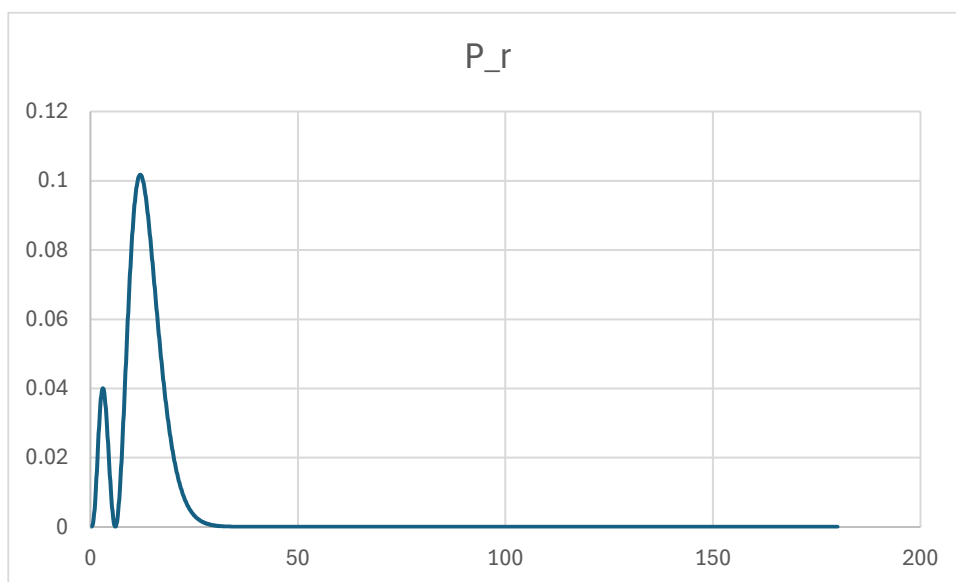


Figure 17 Radial Electron Probability Distribution Function for $Z = 1, n = 3, l = 1, a_0 = 1$

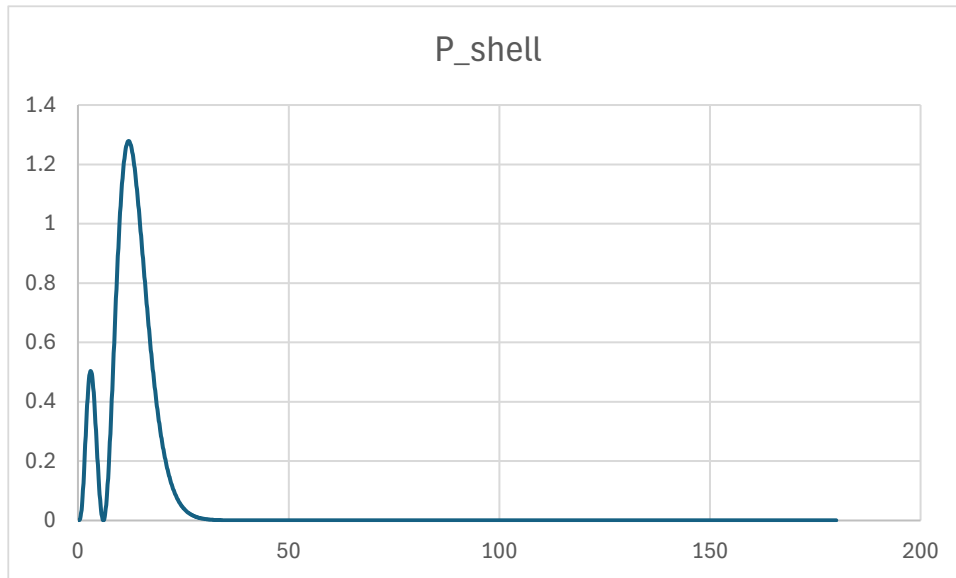


Figure 18 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 3$, $l = 1$, $a_0 = 1$

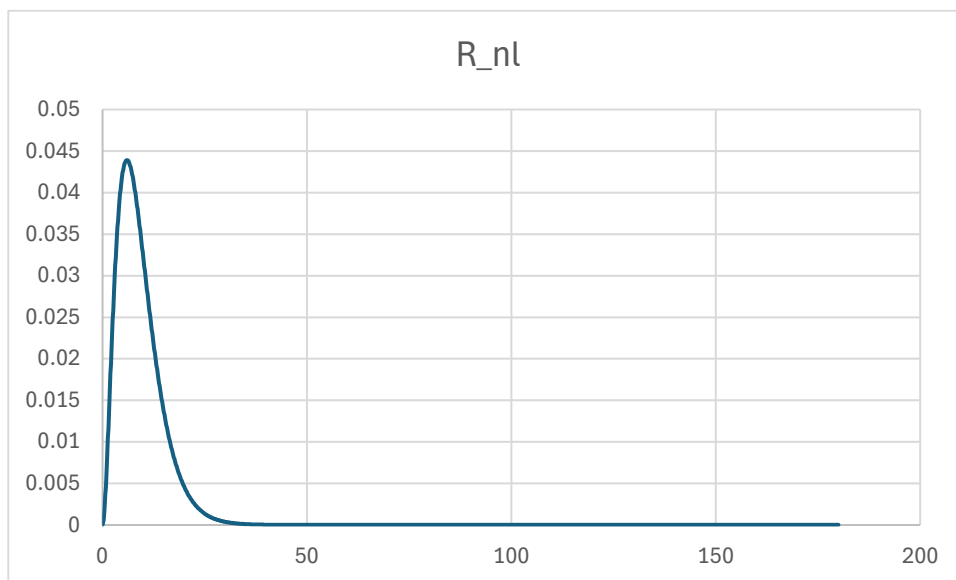


Figure 19 $R_{nl}(r)$ for $Z = 1$, $n = 3$, $l = 2$, $a_0 = 1$

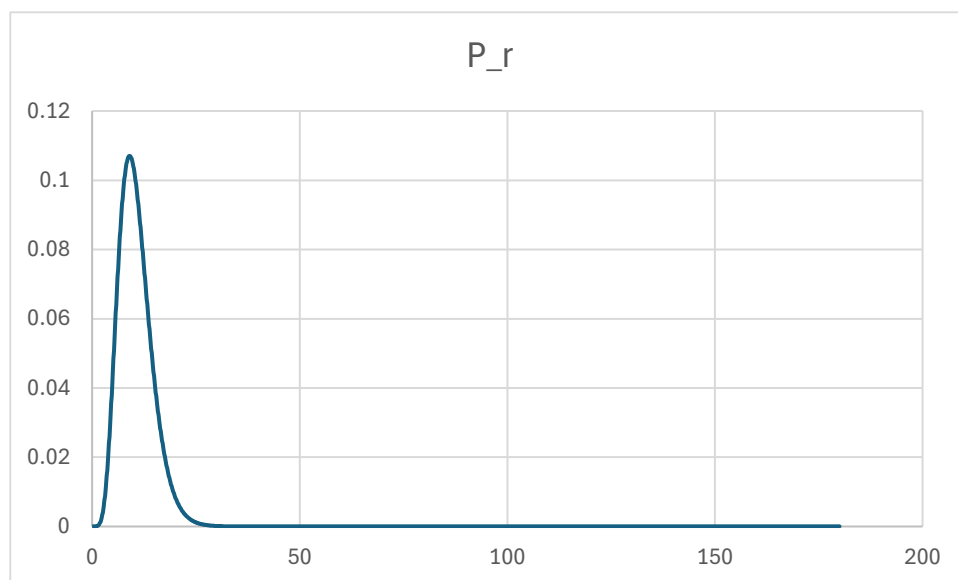


Figure 20 Radial Electron Probability Distribution Function for $Z = 1$, $n = 3$, $l = 2$, $a_0 = 1$

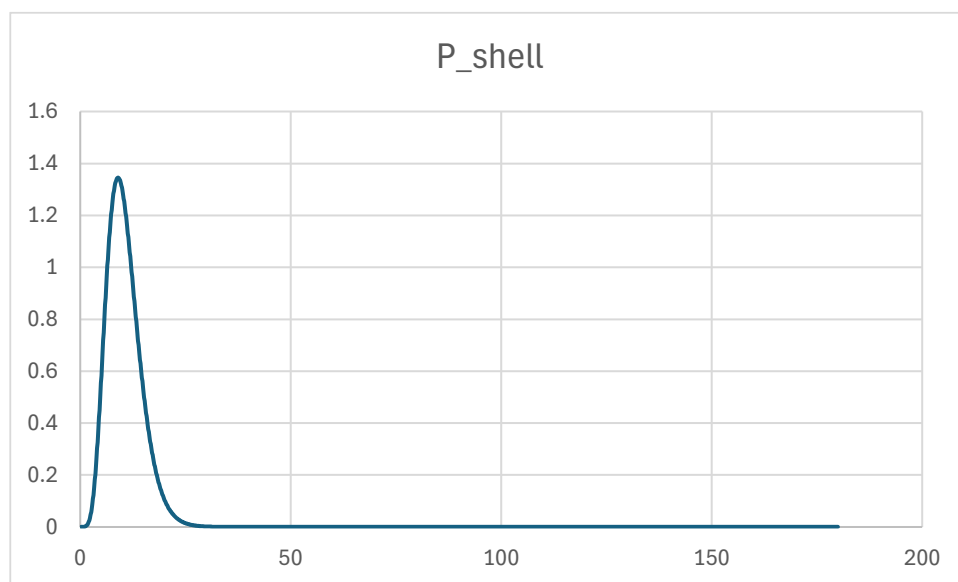


Figure 21 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 3$, $l = 2$, $a_0 = 1$

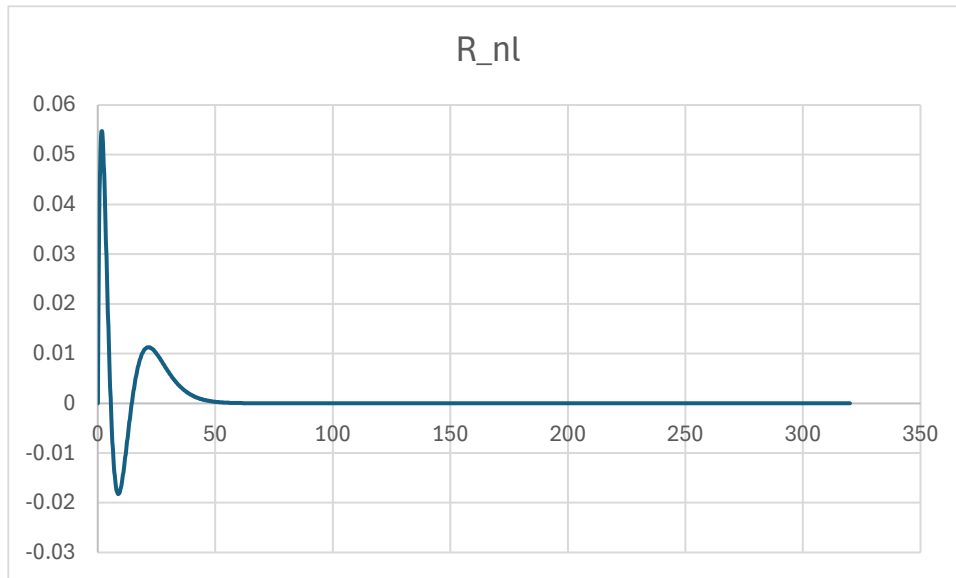


Figure 22 $R_{nl}(r)$ for $Z = 1$, $n = 4$, $l = 0$, $a_0 = 1$

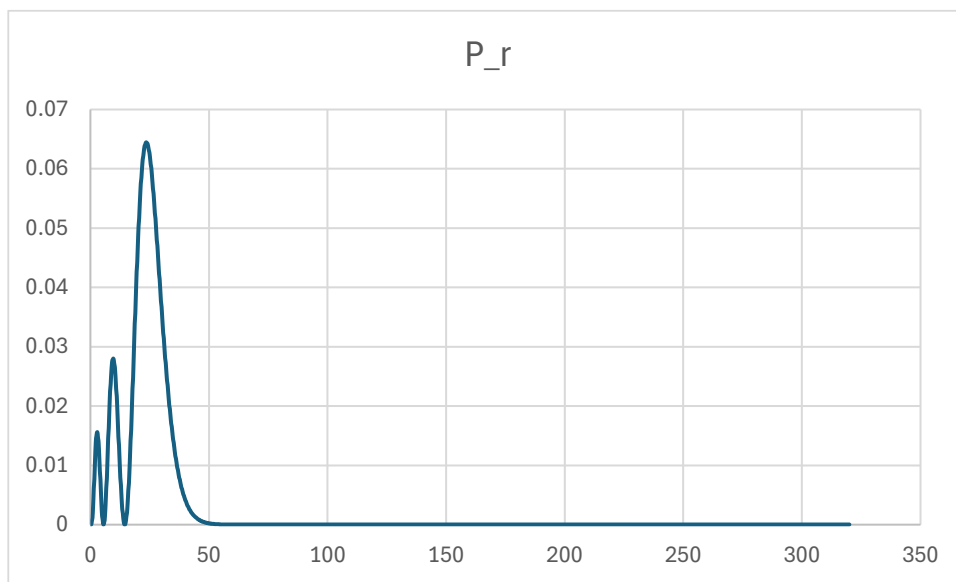


Figure 23 Radial Electron Probability Distribution Function for $Z = 1$, $n = 4$, $l = 0$, $a_0 = 1$

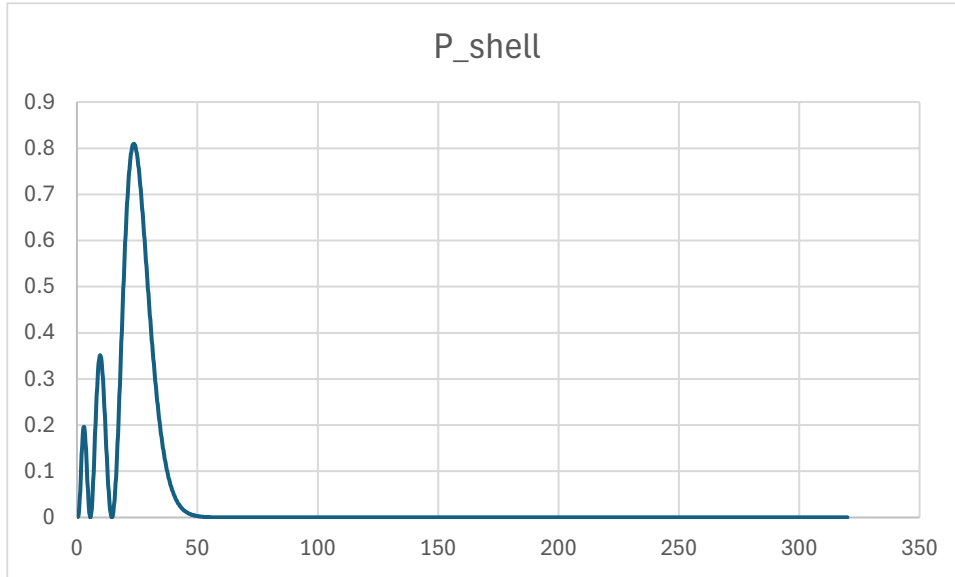


Figure 24 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 4$, $l = 0$, $a_0 = 1$

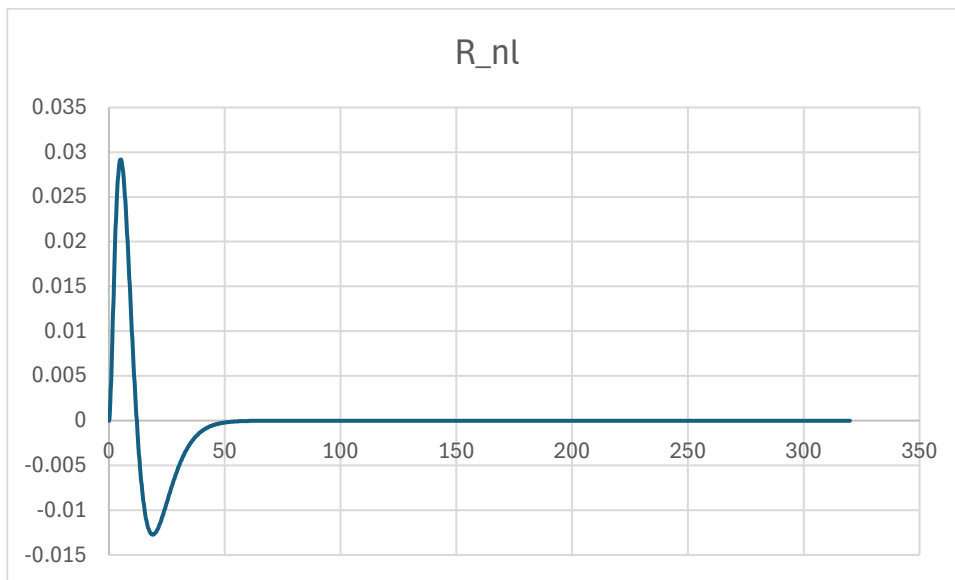


Figure 25 $R_{nl}(r)$ for $Z = 1$, $n = 4$, $l = 1$, $a_0 = 1$

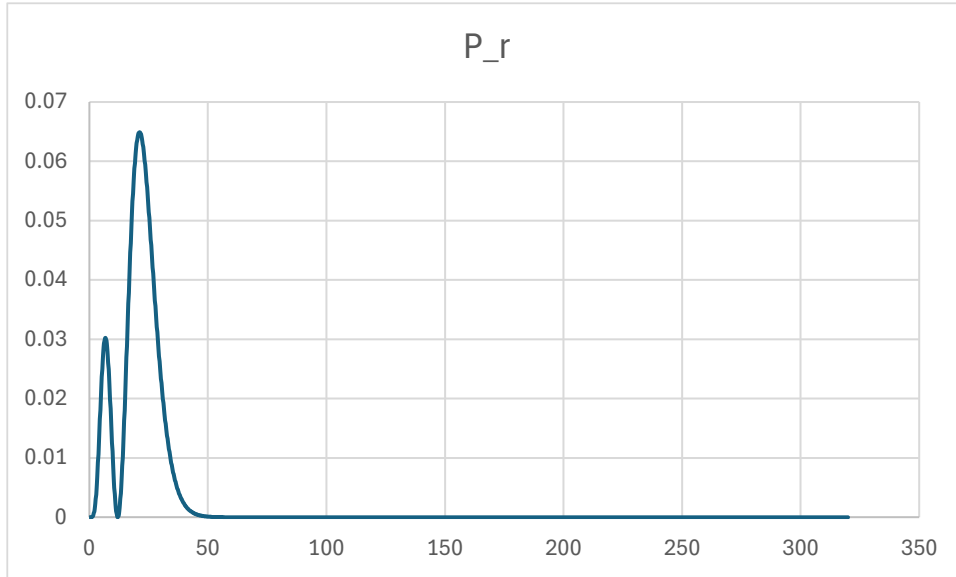


Figure 26 Radial Electron Probability Distribution Function for $Z = 1, n = 4, l = 1, a_0 = 1$

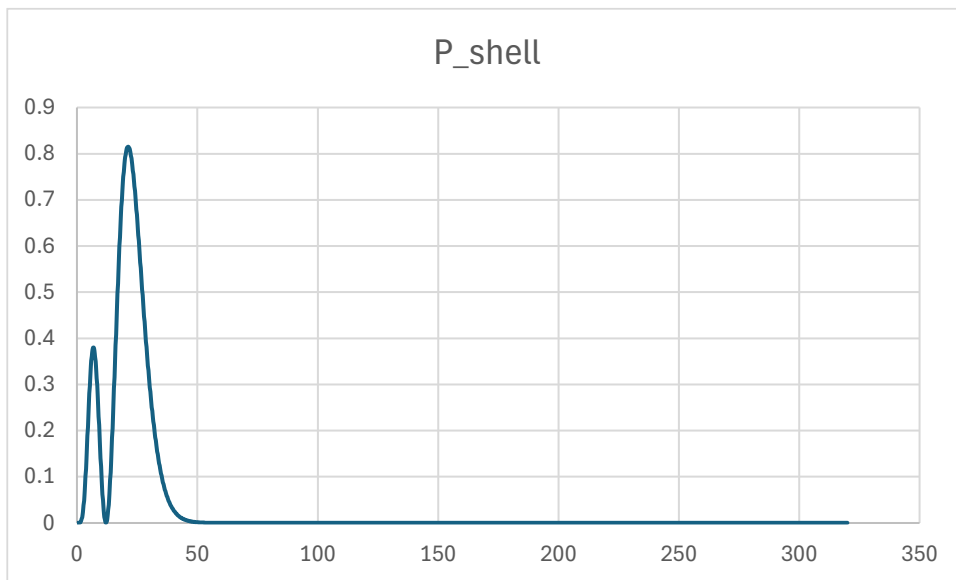


Figure 27 Radial Electron Probability Distribution Shell Function for $Z = 1, n = 4, l = 1, a_0 = 1$

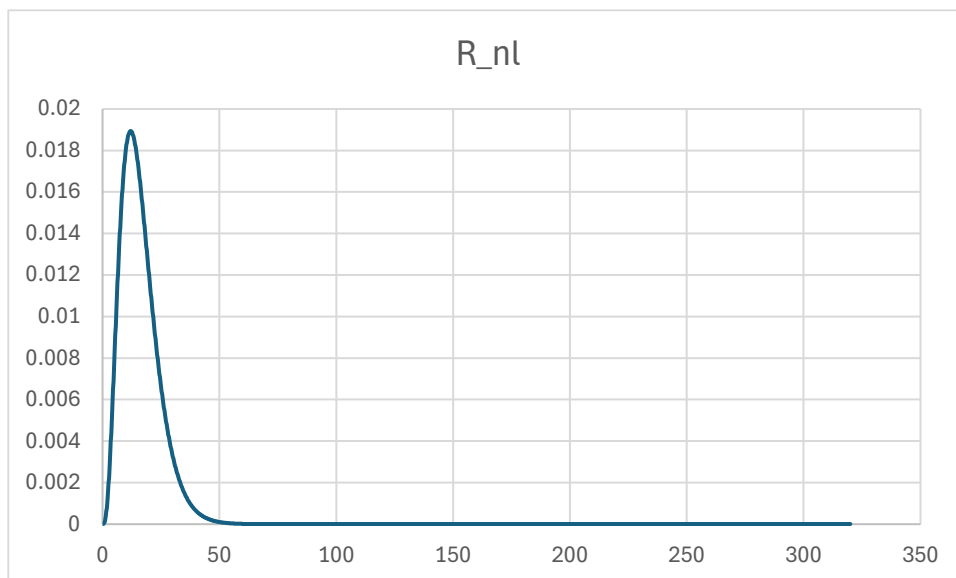


Figure 28 $R_{nl}(r)$ for $Z = 1$, $n = 4$, $l = 2$, $a_0 = 1$

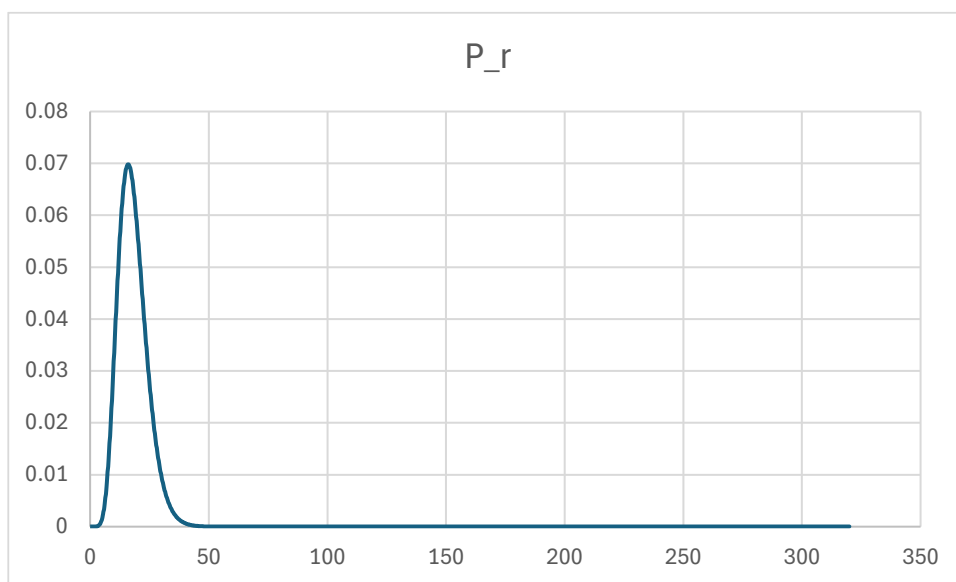


Figure 29 Radial Electron Probability Distribution Function for $Z = 1$, $n = 4$, $l = 2$, $a_0 = 1$

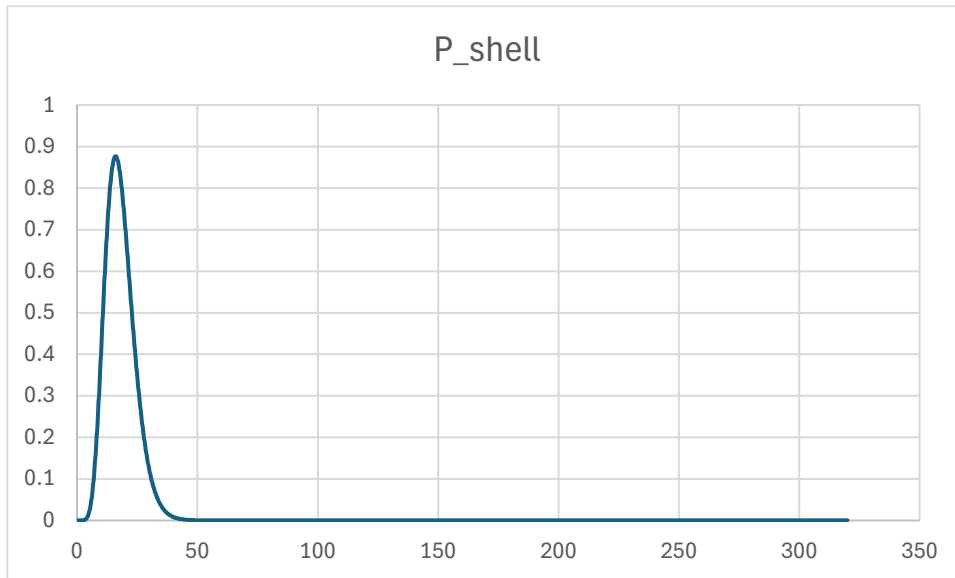


Figure 30 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 4$, $l = 2$, $a_0 = 1$

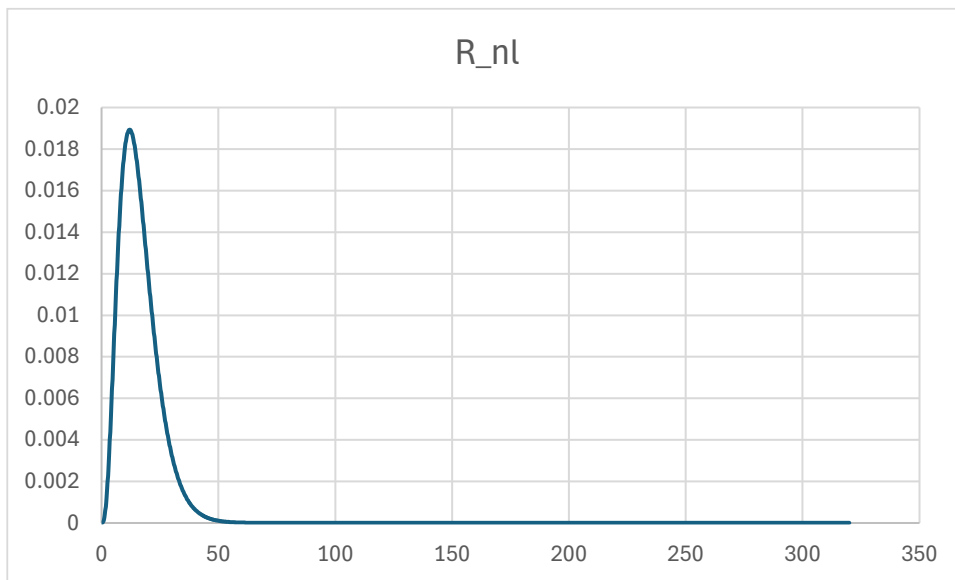


Figure 31 $R_{nl}(r)$ for $Z = 1$, $n = 4$, $l = 3$, $a_0 = 1$

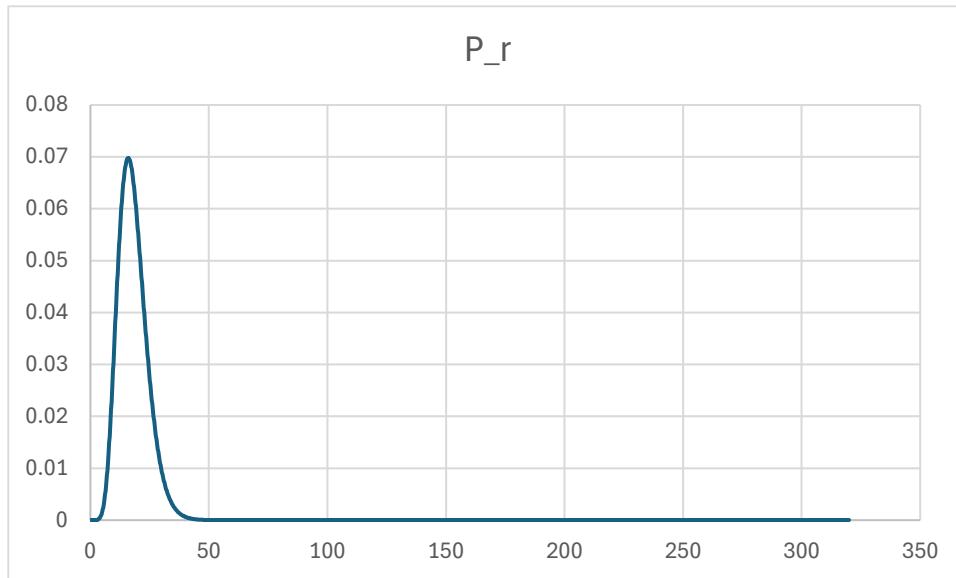


Figure 32 Radial Electron Probability Distribution Function for $Z = 1$, $n = 4$, $l = 3$, $a_0 = 1$

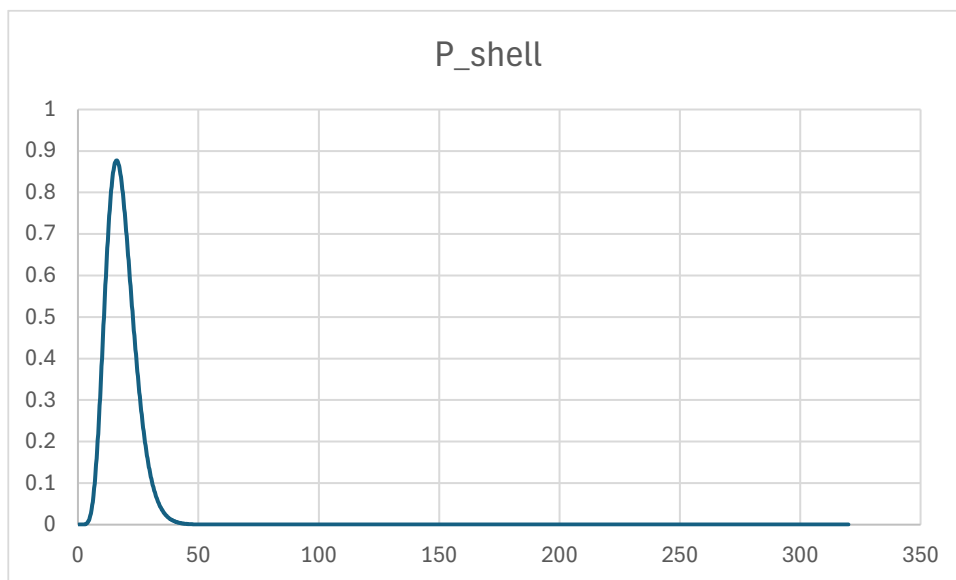


Figure 33 Radial Electron Probability Distribution Shell Function for $Z = 1$, $n = 4$, $l = 3$, $a_0 = 1$

Python source code created by Microsoft's Copilot

```
import numpy as np
import pandas as pd

from math import factorial
from scipy.special import eval_genlaguerre #
generalized/associated Laguerre
```

```

# SciPy docs: eval_genlaguerre(n, alpha, x) evaluates
L_n^{(alpha)}(x) [5] (https://docs.scipy.org/doc/scipy/reference
/generated/scipy.special.eval_genlaguerre.html)

# --- Constants ---
#a0 = 5.29177210903e-11
a0 = 1.0
# Bohr radius in meters (CODATA value; you can treat as a0=1 in
atomic units)

def R_nl(r, n, l, Z, a0_m=a0):
    """
    Hydrogen-like atom radial wavefunction R_{n l}(r) for
    Schrödinger hydrogenic orbitals.
    r: numpy array (meters)
    n: principal quantum number (1,2,3,...)
    l: azimuthal quantum number (0..n-1)
    Z: nuclear charge (Z=1 hydrogen, Z=2 He+, ...)
    Returns R_{n l}(r) in units of 1/sqrt(m^3).
    """
    if n < 1 or l < 0 or l > n - 1:
        raise ValueError("Require n>=1 and 0<=l<=n-1")

    rho = 2.0 * Z * r / (n * a0_m) # dimensionless
    k = n - l - 1 # Laguerre degree
    alpha = 2*l + 1 # Laguerre parameter

    # Normalization prefactor from standard hydrogenic
    solution [1] (https://faculty.washington.edu/seattle/physics441/
    ch10b.pdf)
    pref = (2.0*Z/(n*a0_m))**1.5 * np.sqrt(factorial(n-1-1) /
    (2.0*n*factorial(n+1)))

    # Associated/generalized Laguerre polynomial
    L_{k}^{(alpha)}(rho) [2] (https://en.wikipedia.org/wiki/Laguerre
    _polynomials) [5] (https://docs.scipy.org/doc/scipy/reference/gene
    rated/scipy.special.eval_genlaguerre.html)
    L = eval_genlaguerre(k, alpha, rho)

    return pref * np.exp(-rho/2.0) * (rho**l) * L

def radial_probability_density(r, n, l, Z, a0_m=a0):
    """
    Radial probability density P_{n l}(r) = r^2 |R_{n l}(r)|^2.
    (Many texts also plot 4π r^2 |R|^2; see function below.)
    """
    R = R_nl(r, n, l, Z=Z, a0_m=a0_m)

```

```

    return (r**2) * (np.abs(R)**2)

def radial_shell_probability_density(r, n, l, Z, a0_m=a0):
    """
    Probability density per spherical shell:  $4\pi r^2 |R_{nl}(r)|^2$ .
    This corresponds to multiplying by the surface area  $4\pi r^2$  of
    a shell.
    [3] (https://ch301.cm.utexas.edu/section2.php?target=atomic/H-atom/radial-distribution.html)
    """
    R = R_nl(r, n, l, Z, a0_m=a0_m)
    return 4.0*np.pi*(r**2)*(np.abs(R)**2)

def demo_plot(n, l, Z, rmax_in_a0=None, num=4000):
    if rmax_in_a0 is None:
        rmax_in_a0 = 20.0 * (n**2) / max(Z, 1)

    r = np.linspace(0.0, rmax_in_a0*a0, num)
    R = R_nl(r, n, l, Z)

    # Call positionally to avoid any keyword-arg mismatch in
    some frontends
    P = radial_probability_density(r, n, l, Z)
    P_shell = radial_shell_probability_density(r, n, l, Z)

    fig, axs = plt.subplots(3, 1, figsize=(8, 10), sharex=True)

    axs[0].plot(r/a0, R)
    axs[0].set_ylabel(r"$R_{n\ell}(r)$")
    axs[0].grid(True)

    axs[1].plot(r/a0, P)
    axs[1].set_ylabel(r"$r^2 |R_{n\ell}(r)|^2$")
    axs[1].grid(True)

    axs[2].plot(r/a0, P_shell)
    axs[2].set_ylabel(r"$4\pi r^2 |R_{n\ell}(r)|^2$")
    axs[2].set_xlabel(r"$r/a_0$")
    axs[2].grid(True)

    fig.suptitle(f"Hydrogen-like radial functions: n={n}, l={l},
Z={Z}")
    fig.tight_layout()
    plt.show()
    df = pd.DataFrame({
        "r/a0": r/a0,

```

```

    "R_nl": R,
    "P_r": P,
    "P_shell": P_shell
  })

  df

# Example usage
# print(os.getcwd())
Z_raw = xl("B1")          # Excel -> Python (may come in as a
small table-like object)
#Z = int(np.array(Z_raw).ravel()[0]) # robustly #extract the
scalar and #convert to int
#n_raw = xl("C1")         # Excel -> Python (may come #in as a
small table-like #object)
#n = int(np.array(n_raw).ravel()[0]) # robustly #extract the
scalar and #convert to int
#l_raw = xl("D1")        # Excel -> Python (may come #in as a
small table-like #object)
#l = int(np.array(l_raw).ravel()[0]) # robustly #extract the
scalar and #convert to int
import pandas as pd
import numpy as np

# Read scalars from Excel cells
Z = int(np.array(xl("B1")).ravel()[0])
n = int(np.array(xl("C1")).ravel()[0])
l = int(np.array(xl("D1")).ravel()[0])

# Define r-grid HERE (so r is defined in the main scope)
rmax_in_a0 = 20.0 * (n**2) / max(Z, 1)
r = np.linspace(0.0, rmax_in_a0*a0, 2000)

# Compute arrays
R = R_nl(r, n, l, Z)
P = radial_probability_density(r, n, l, Z)
P_shell = radial_shell_probability_density(r, n, l, Z)

# Return a DataFrame (make this the last line so it spills into
Excel)
pd.DataFrame({
    "r_over_a0": r/a0,
    "R_nl": R,
    "P_r": P,
    "P_shell": P_shell
})
# demo_plot(n=2, l=0, Z=1)

```

```
# demo_plot(n=2, l=1, z=1)
```

References

- [1] A. Boehm, "VII Alkali Atoms and the Schroedinger Equation of One-Electron Atoms," in *Quantum Mechanics*, New York, Springer-Verlog New York Inc., 1979, pp. 189-206.
- [2] E. Merzbacher, "10. Piecewise Constant Potentials in Three Dimensions and the Hydrogen Atom," in *Quantum Mechanics Second Edition*, New York, John Wiley & Sons Inc., 1970, pp. 80-115.
- [3] A. Messiah, "Chapter XI The Coulomb Interaction 1. The Hydrogen Atom," in *Quantum Mechanics Two Volumes Bound as One*, Mineola, Dover Publications, Inc., 2014, pp. 412-420.
- [4] L. I. Schiff, "Hydrogen-Atom Wave Functions," in *Quantum Mechanics Third Edition*, New York, McGraw-Hill, Inc, 1968, pp. 93-94.
- [5] P. Linus and J. E. B. Wilson, "Introduction to Quantum Mechanics with Applications to Chemistry Kindle Edition," [Online]. Available: <https://amazon.com>. [Accessed 25 May 2026].