HYDROGEN ATOM: RADIAL FUNCTIONS FOR LARGE L

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.46.

In solving the radial equation for the hydrogen atom, we arrived at the solution

$$u(\rho) = \rho^{l+1}e^{-\rho}v(\rho) \tag{1}$$

$$u(r) \equiv rR(r) \tag{2}$$

$$\rho = \kappa r \tag{3}$$

$$\rho_0 = \frac{me^2}{2\pi\varepsilon_0\hbar^2\kappa} \tag{4}$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \tag{5}$$

with $v(\rho)$ given by a series

$$v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j \tag{6}$$

The coefficients turned out to satisfy the recursion formula

$$c_{j+1} = \frac{2(j+l+1)-2n}{(j+1)(j+2(l+1))}c_j \tag{7}$$

For $l = n-1$, the recursion formula becomes

$$c_{j+1} = \frac{2j}{(j+1)(j+2n)}c_j \tag{8}$$

where we need to specify c_0 to get the series started. Working back to the radial function gives us

$$R_{n(n-1)}(r) = \frac{c_0}{(an)^n}r^{n-1}e^{-r/an} \tag{9}$$

We can combine the constant out front into a single constant $N_n = c_0/(an)^n$.

To normalize, we evaluate the integral (using software)

$$\int_0^\infty R^2_{n(n-1)}(r)dr = \frac{c_0^2}{(an)^{2n}} \int_0^\infty r^{2(n-1)} e^{-2r/an} r^2 dr \tag{10}$$

$$= \frac{na(2n)!}{2^{2n+1}} c_0^2 \tag{11}$$

$$= 1 \tag{12}$$

$$c_0 = 2^n \sqrt{\frac{2}{an(2n)!}} \tag{13}$$

$$N_n = 2^n \sqrt{\frac{2}{(an)^{2n+1}(2n)!}} \tag{14}$$

Expectation values are calculated in the usual way:

$$\langle r \rangle = \frac{2^{2n+1}}{(an)^{2n+1}(2n)!} \int_0^\infty r^{2(n-1)+3} e^{-2r/an} dr \tag{15}$$

$$= \frac{(2n+1)na}{2} \tag{16}$$

$$\langle r^2 \rangle = \frac{2^{2n+1}}{(an)^{2n+1}(2n)!} \int_0^\infty r^{2(n-1)+4} e^{-2r/an} dr \tag{17}$$

$$= \frac{(n+1)(2n+1)n^2a^2}{2} \tag{18}$$

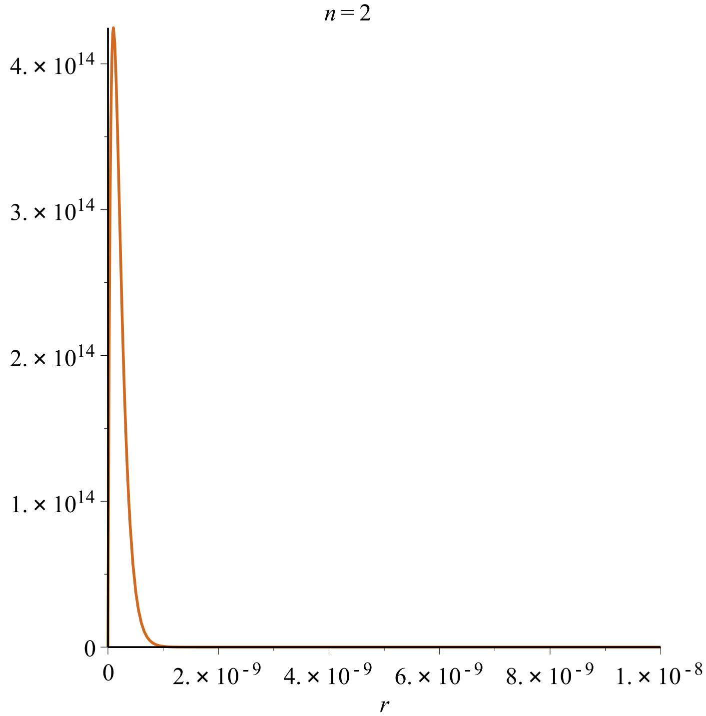
$$\sigma_r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} \tag{19}$$

$$= \frac{na\sqrt{2n+1}}{2} \tag{20}$$

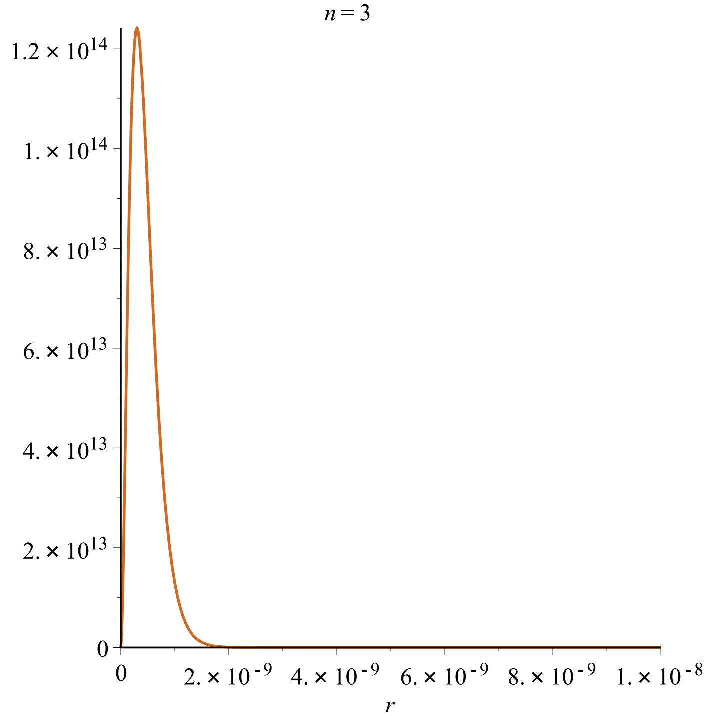
$$= \frac{\langle r \rangle}{\sqrt{2n+1}} \tag{21}$$

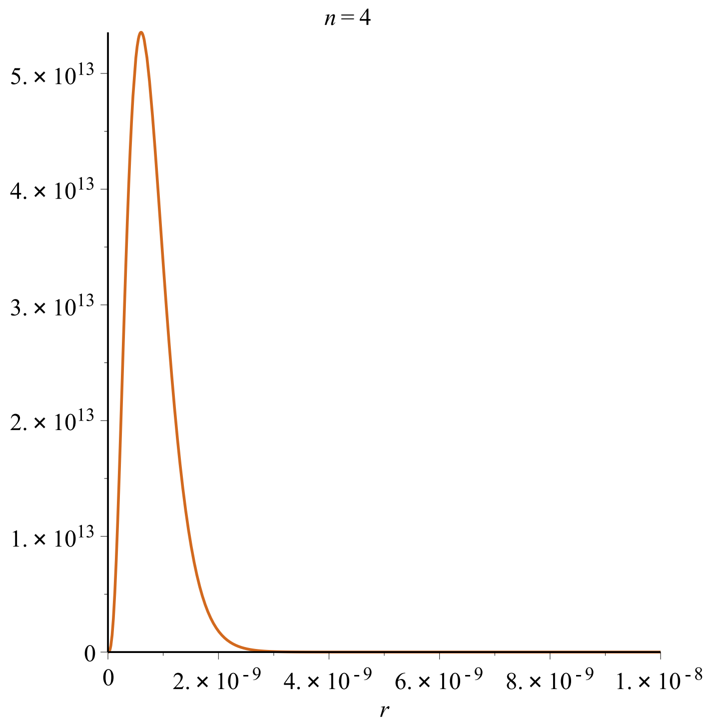
A few radial functions $R_{n(n-1)}(r)$ are shown. The domain of r is up to $200a$ in each case.

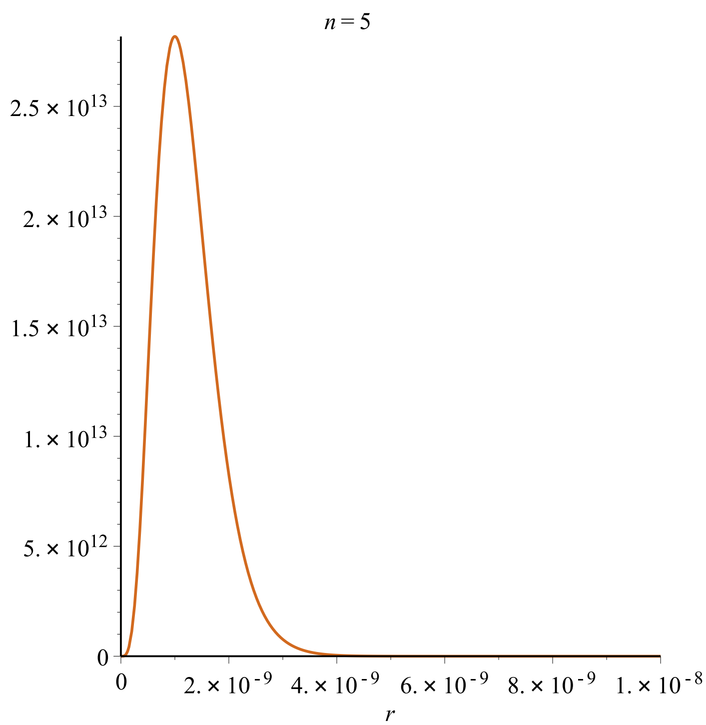
$n = 2$

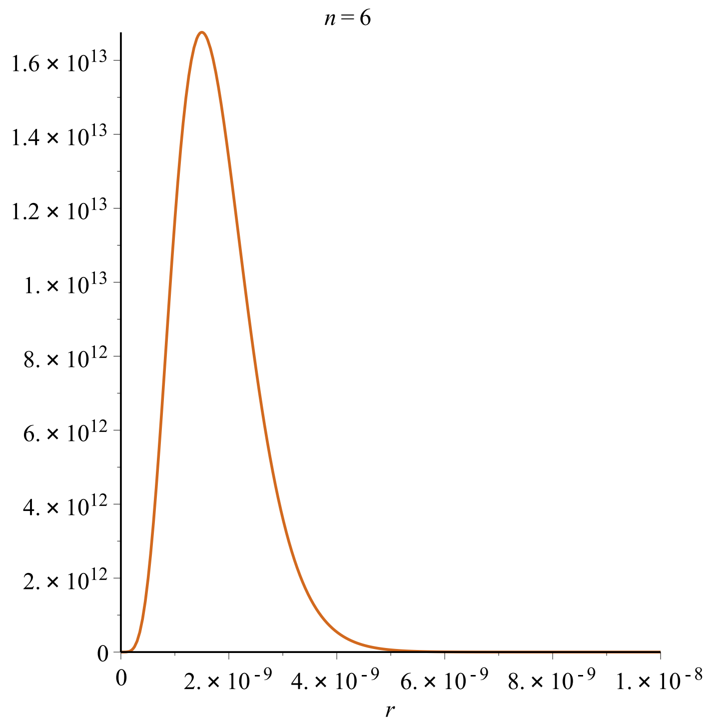

4. × 10^14
3. × 10^14
2. × 10^14
1. × 10^14
0
0
2. × 10^-9
4. × 10^-9
6. × 10^-9
8. × 10^-9
1. × 10^-8
r

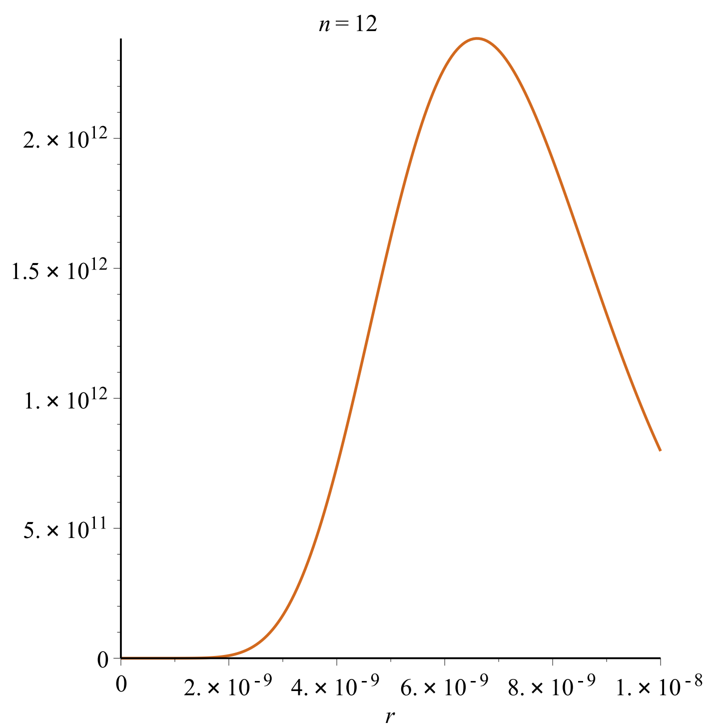
$n = 3$


1.2 × 10^14
1. × 10^14
8. × 10^13
6. × 10^13
4. × 10^13
2. × 10^13
0
0
2. × 10^-9
4. × 10^-9
6. × 10^-9
8. × 10^-9
1. × 10^-8
r


n = 4
5. × 10^13
4. × 10^13
3. × 10^13
2. × 10^13
1. × 10^13
0
0
2. × 10^-9
4. × 10^-9
6. × 10^-9
8. × 10^-9
1. × 10^-8
r


n = 5
2.5 × 10^13
2. × 10^13
1.5 × 10^13
1. × 10^13
5. × 10^12
0
0
2. × 10^-9
4. × 10^-9
6. × 10^-9
8. × 10^-9
1. × 10^-8
r


$n = 6$
1.6×10^{13}
1.4×10^{13}
1.2×10^{13}
$1. \times 10^{13}$
$8. \times 10^{12}$
$6. \times 10^{12}$
$4. \times 10^{12}$
$2. \times 10^{12}$
0
0
$2. \times 10^{-9}$
$4. \times 10^{-9}$
$6. \times 10^{-9}$
$8. \times 10^{-9}$
$1. \times 10^{-8}$
r


$n = 12$
$2. \times 10^{12}$
1.5×10^{12}
$1. \times 10^{12}$
$5. \times 10^{11}$
0
0
$2. \times 10^{-9}$
$4. \times 10^{-9}$
$6. \times 10^{-9}$
$8. \times 10^{-9}$
$1. \times 10^{-8}$
r