

Radial wave function of hydrogen-like atom
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date February, 21, 2013)

1. The radial wave function for a hydrogen-like atom.

$$R_{nl}(r) = \sqrt{\frac{4Z^3(n-l-1)!}{a^3 n^4 (n+l)!}} e^{-\frac{Zr}{na}} \left(\frac{2Zr}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2Zr}{na}\right)$$

where

$$\int_0^\infty dr r^2 [R_{nl}(r)]^2 = 1 \quad \text{(the normalization condition)}$$

and

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

For the hydrogen atom, we have $Z = 1$ and $\mu = m$. $a = a_B$ (Bohr radius).

((Mathematica))

	$\ell=0$	$\ell=1$	$\ell=2$
$n=1$	$\frac{2}{a^{3/2}} e^{-\frac{r}{a}}$		
$n=2$	$\frac{1}{2\sqrt{2}a^{5/2}} e^{-\frac{r}{2a}} (2a-r)$	$\frac{1}{2\sqrt{6}a^{5/2}} e^{-\frac{r}{2a}} r$	
$n=3$	$\frac{2}{81\sqrt{3}a^{7/2}} e^{-\frac{r}{3a}} (27a^2 - 18ar + 2r^2)$	$\frac{4}{81a^{7/2}} e^{-\frac{r}{3a}} r (6a-r)$	$\frac{2}{81a^{7/2}} e^{-\frac{r}{3a}} r^2$

((Laguerre polynomials))

$L_{n-l-1}^{2l+1}(x)$ is the associated Laguerre polynomial.

n	$l = 0$	$l = 1$	$l = 2$	$l = 3$
1	1			
2	$2-x$	1		
3	$\frac{1}{2}(6-6x+x^2)$	$4-x$	1	
4	$\frac{1}{6}(24-36x+12x^2-x^3)$	$\frac{1}{2}(20-10x+x^2)$	$6-x$	1

((Mathematica))

	$\ell=0$	$\ell=1$	$\ell=2$	$\ell=3$	$\ell=4$
n=1	1				
n=2	$2-x$	1			
n=3	$\frac{1}{2}(6-6x+x^2)$	$4-x$	1		
n=4	$\frac{1}{6}(24-36x+12x^2-x^3)$	$\frac{1}{2}(20-10x+x^2)$	$6-x$	1	
n=5	$\frac{1}{24}(120-240x+120x^2-20x^3+x^4)$	$\frac{1}{6}(120-90x+18x^2-x^3)$	$\frac{1}{2}(42-14x+x^2)$	$8-x$	1

2. ($n = 1$ and $l = 0$) 1s state

The radial wave function is given by

$$R_{1,0} = \frac{2Z^{3/2}}{a^{3/2}} e^{-\frac{rZ}{a}}.$$

The probability density distribution $P(r)$ is defined by

$$P(r) = r^2 R_{1,0}^2 = \frac{4Z^3}{a^3} r^2 e^{-\frac{2rZ}{a}},$$

where $R_{1,0}^2$ is called the probability density and

$$P(r)dr = dr r^2 R_{1,0}^2$$

is the probability for finding the electron in this state between r and $r+dr$. Note that

$$\int_0^{\infty} dr P(r) = 1.$$

Since

$$\frac{d}{dr} P(r) = \frac{8Z^3}{a^4} r e^{-\frac{2rZ}{a}} (a - rZ),$$

$P(r)$ shows a peak at $r = \frac{a}{Z}$. The average of r is given by

$$\langle r \rangle = \int_0^{\infty} dr r P(r) = \int_0^{\infty} dr r^3 R_{1,0}^2 = \frac{3a}{2Z}.$$

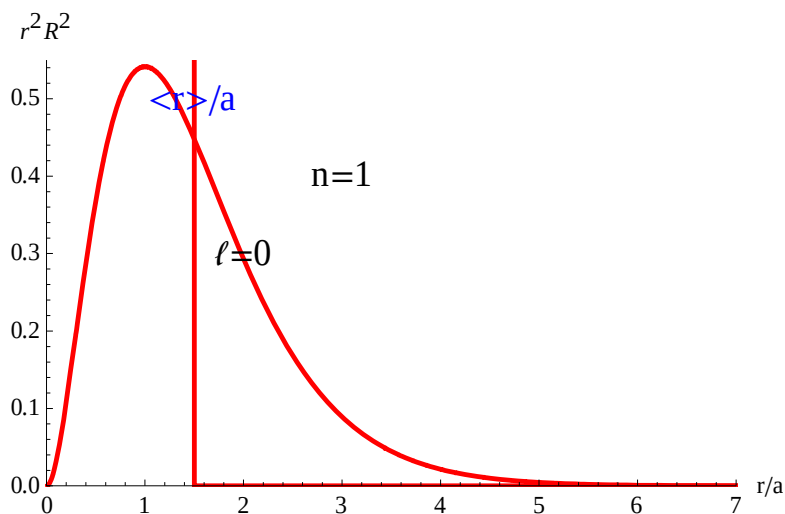


Fig. Radial probability distribution $P(r)$ for the ground state of hydrogen. $a = a_B$. $Z = 1$. $\mu = m$.

The cumulative probability density:

$$\int_0^r P(r) dr = 1 - e^{-\frac{2rZ}{a}} \left[1 + 2Z\left(\frac{r}{a}\right) + 2Z^2\left(\frac{r}{a}\right)^2 \right].$$

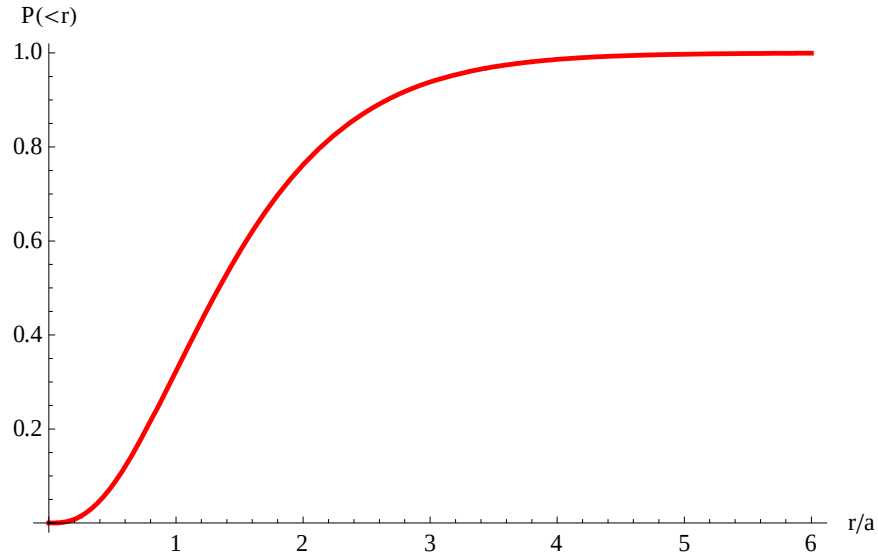


Fig. Cumulative probability density for the 2s state of hydrogen atom. $a = a_B$. $Z = 1$. $\mu = m$.

Average and uncertainty:

$$\langle r^p \rangle = \int_0^{\infty} dr r^p P(r) = \frac{1}{2^{p+1}} \left(\frac{a}{Z}\right)^p (p+2)!,$$

where p is integer;

$$\langle r^2 \rangle = \frac{1}{2^3} \left(\frac{a}{Z}\right)^2 4! = 3 \left(\frac{a}{Z}\right)^2.$$

The standard deviation:

$$\frac{\sqrt{\langle r^2 \rangle - \langle r \rangle^2}}{\langle r \rangle} = \frac{1}{\sqrt{3}}.$$

((Mathematica))

Hydrogenic atom: Radial wave function
1s state (ground state)

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Clear["Global`*"];
rwave[n_, l_, r_] :=
  1 / (Sqrt[n + l]!)
  (21+l a-l-3/2 e-Zr/a n-l-2 Zl+3/2 rl Sqrt[n - l - 1]!
    LaguerreL[-1 + n - l, 1 + 2 l, (2 Z r) / (a n)])];
average[n_, l_] :=
  a / (2 Z (3 n2 - l (l + 1))) /. {a -> 1, Z -> 1};
h[n_, l_, r_] := Which[0 < r < average[n, l],
  1, r > average[n, l], 0]
p11[n_] :=
  Plot[
    Evaluate[
      Table[r2 rwave[n, l, r]^2 /. {a -> 1, Z -> 1},
        {l, 0, n - 1}], {r, 0.01, 7 n},
    PlotStyle -> Table[{{Thick, Hue[0.2 i]}},
      {i, 0, 10}],
    PlotRange -> {{0, 7 n}, {0, 0.55 1/n1.2}},
    AxesLabel -> {"r/a", "r2R2"}];
p12[n_] :=
  Plot[Evaluate[Table[h[n, l, r], {l, 0, n - 1}]],
    {r, 0.01, 7 n},
    PlotStyle -> Table[{{Thick, Hue[0.2 i]}},
      {i, 0, 10}], PlotRange -> {{0, 7 n}, {0, 1}},
    AxesLabel -> {"r/a", "Pr"}];
g1 =
  Graphics[
    {Text[Style["n=1", Black, 15], {3, 0.4}],
      Text[Style["l=0", Black, 15], {2, 0.3}],
      Text[Style["<r>/a", Blue, 15], {1.5, 0.5}]}];

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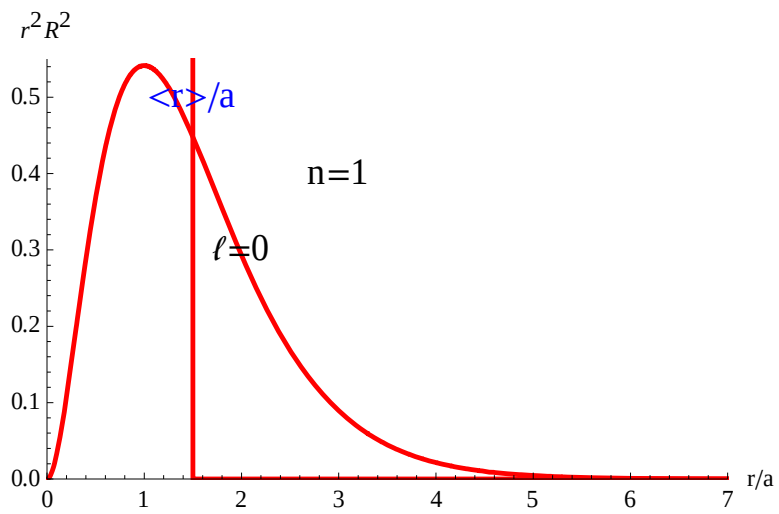
`rwave[n, ℓ, r] /. {n → 1, ℓ → 0}`

$$\frac{2 e^{-\frac{r Z}{a}} Z^{3/2}}{a^{3/2}}$$

`P1 = r2 rwave[n, ℓ, r]^2 /. {n → 1, ℓ → 0}`

$$\frac{4 e^{-\frac{2 r Z}{a}} r^2 Z^3}{a^3}$$

`Show[p11[1], p12[1], g1]`



D[P1, r] // Simplify

$$\frac{8 e^{-\frac{2 r Z}{a}} r Z^3 (a - r Z)}{a^4}$$

Average and standard deviation (uncertainty)

K[p_] = Integrate[r^p P1, {r, 0, ∞}] // Simplify[#, {p > -3, Re[$\frac{Z}{a}$] > 0}] &;

**Table[K[p], {p, -2, 3}] // TableForm[#,
TableHeadings → {"p=-2", "p=-1", "p=0", "p=1", "p=2", "p=3"}]] &**

p=-2	$\frac{2 Z^2}{a^2}$
p=-1	$\frac{Z}{a}$
p=0	1
p=1	$\frac{3 a}{2 Z}$
p=2	$\frac{3 a^2}{Z^2}$
p=3	$\frac{15 a^3}{2 Z^3}$

k12 = $\sqrt{K[2] - K[1]^2}$ // Simplify

$$\frac{1}{2} \sqrt{3} \sqrt{\frac{a^2}{Z^2}}$$

$\frac{k12}{K[1]}$ // Simplify[#, {Z > 0, a > 0}] &

$$\frac{1}{\sqrt{3}}$$

K[p]

$$2^{-1-p} \left(\frac{Z}{a}\right)^{-p} \text{Gamma}[3 + p]$$

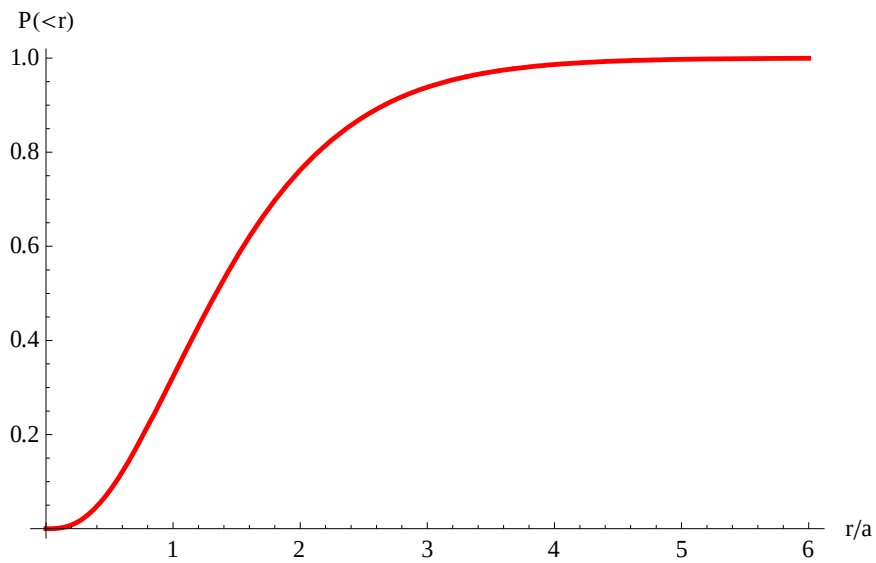
Cumulative probability

g1 = Integrate[P1, {r, 0, r}] // Simplify

$$1 - \frac{e^{-\frac{2 r Z}{a}} (a^2 + 2 a r Z + 2 r^2 Z^2)}{a^2}$$

```
g11 = g1 /. {Z -> 1, a -> 1};
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```
Plot[g11, {r, 0, 6}, PlotStyle -> {Red, Thick}, AxesLabel -> {"r/a", "P(<r)"}]
```



3. ($n = 2$ and $l = 0$) 2s state

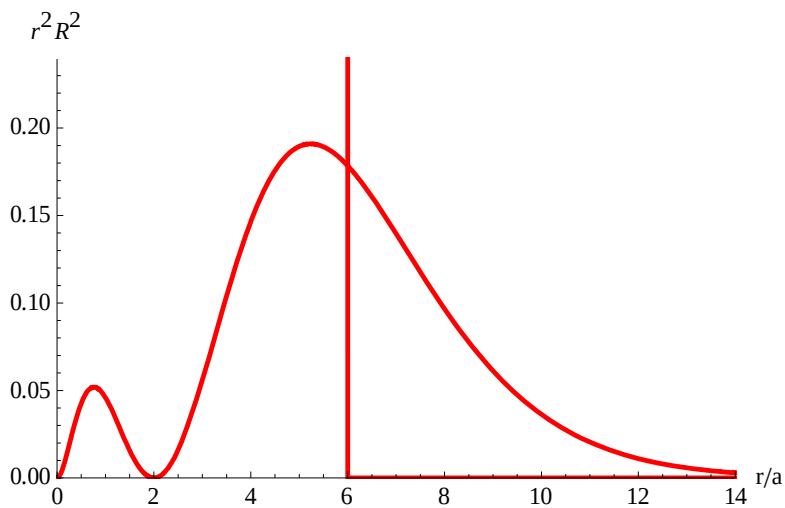


Fig. Radial probability distribution $P(r)$ for the 2s state of hydrogen. $a = a_B$. $Z = 1$. $\mu = m$. The local maxima are at $r/a = 0.7639$, and 5.236 . The local minimum is at $r/a = 0$, and 2 .

The radial wave function:

$$R_{2,0} = \frac{Z^{3/2}}{2\sqrt{2}a^{3/2}} e^{-\frac{rZ}{2a}} \left(2 - \frac{rZ}{a}\right).$$

The probability:

$$P(r) = r^2 R_{2,0}^2 = \frac{Z^3}{8a^3} e^{-\frac{rZ}{a}} r^2 \left(2 - \frac{rZ}{a}\right)^2.$$

Since

$$\frac{d}{dr} P(r) = \frac{Z^3}{8a^6} e^{-\frac{rZ}{a}} r(2a - rZ)(4a^2 - 6arZ + r^2 Z^2),$$

$P(r)$ shows local maxima at

$$r = \frac{(3 - \sqrt{5})a}{Z}, \quad r = \frac{(3 + \sqrt{5})a}{Z}$$

and a local minimum at

$$r = \frac{2a}{Z}$$

The average of r^p is given by

$$\langle r^p \rangle = \int_0^\infty dr r^p P(r) = \left(\frac{4 + 3p + p^2}{8} \right) \left(\frac{a}{Z} \right)^p (p + 2)!$$

For $p = 1$, we have

$$\langle r \rangle = 6 \left(\frac{a}{Z} \right).$$

For $p = 2$, we have

$$\langle r^2 \rangle = 42 \left(\frac{a}{Z} \right)^2$$

The uncertainty for r is

$$\frac{\sqrt{\langle r^2 \rangle - \langle r \rangle^2}}{\langle r \rangle} = \frac{1}{\sqrt{6}}$$

The cumulative probability is

$$\int_0^r P(r) dr = 1 - e^{-\frac{Zr}{a}} \left[1 + \left(\frac{Zr}{a} \right) + \frac{1}{2} \left(\frac{Zr}{a} \right)^2 + \frac{1}{8} \left(\frac{Zr}{a} \right)^4 \right]$$

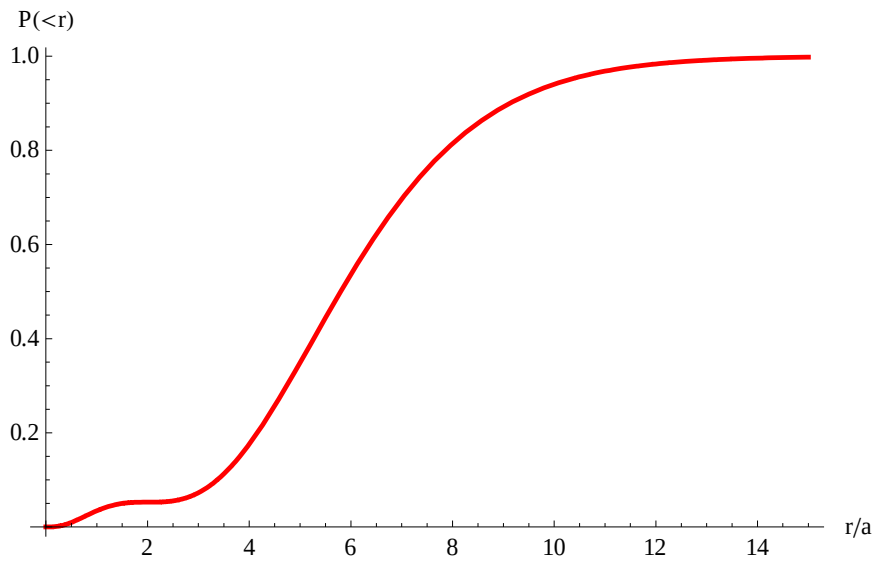


Fig. Cumulative probability density for the 2s state of hydrogen atom. $a = a_B$. $Z = 1$. $\mu = m$.

3. $(n = 3 \text{ and } l = 0)$ 3s state

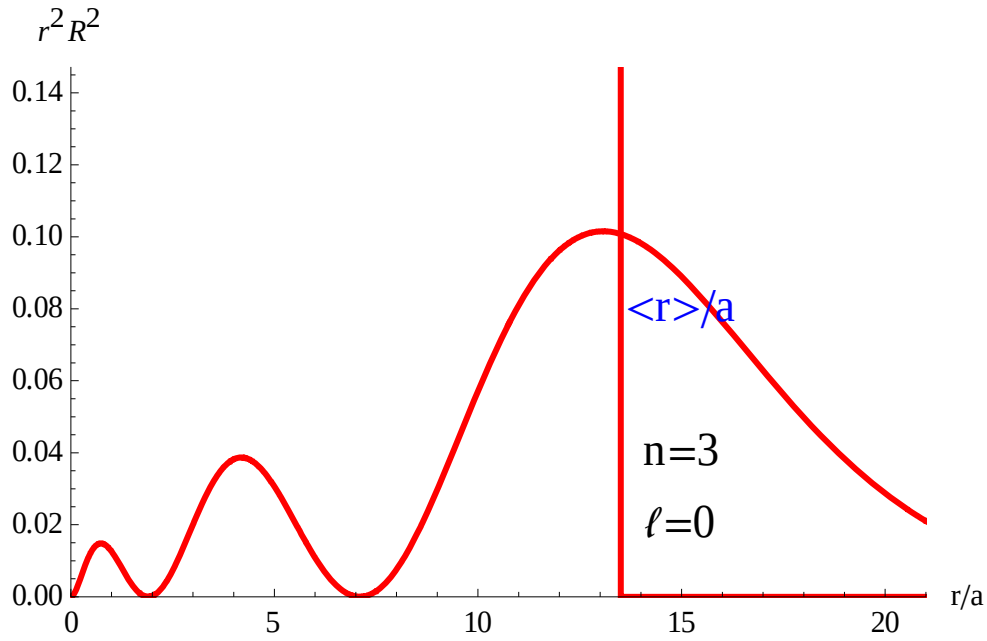


Fig. Radial probability distribution $P(r)$ for the 3s state of hydrogen. $a = a_B$. $Z = 1$. $\mu = m$. The local maxima are at $r/a = 0.740$, 4.186 , and 13.07 . The local minimum is at $r/a = 0$, 1.9019 , 7.098 .

The radial wave function:

$$R_{3,0} = \frac{2Z^{3/2}}{81\sqrt{3}a^{7/2}} e^{-\frac{rZ}{3a}} \left[27 - 18\left(\frac{rZ}{a}\right) + 2\left(\frac{rZ}{a}\right)^2 \right].$$

The probability:

$$P(r) = r^2 R_{3,0}^2.$$

Since

$$\frac{d}{dr} P(r) = 0,$$

$P(r)$ shows local maxima at

$$r = 13.074 \frac{a}{Z}, \quad r = 4.18593 \frac{a}{Z}, \quad r = 0.740037 \frac{a}{Z}$$

The average of r^p is given by

$$\langle r^p \rangle = \int_0^{\infty} dr r^p P(r)$$

For $p = 1$, we have

$$\langle r \rangle = \frac{27}{2} \left(\frac{a}{Z} \right).$$

For $p = 2$, we have

$$\langle r^2 \rangle = 207 \left(\frac{a}{Z} \right)^2$$

The uncertainty for r is

$$\frac{\sqrt{\langle r^2 \rangle - \langle r \rangle^2}}{\langle r \rangle} = \frac{\sqrt{11}}{9}$$

The cumulative probability is

$$P(< r) = \int_0^r P(r) dr$$

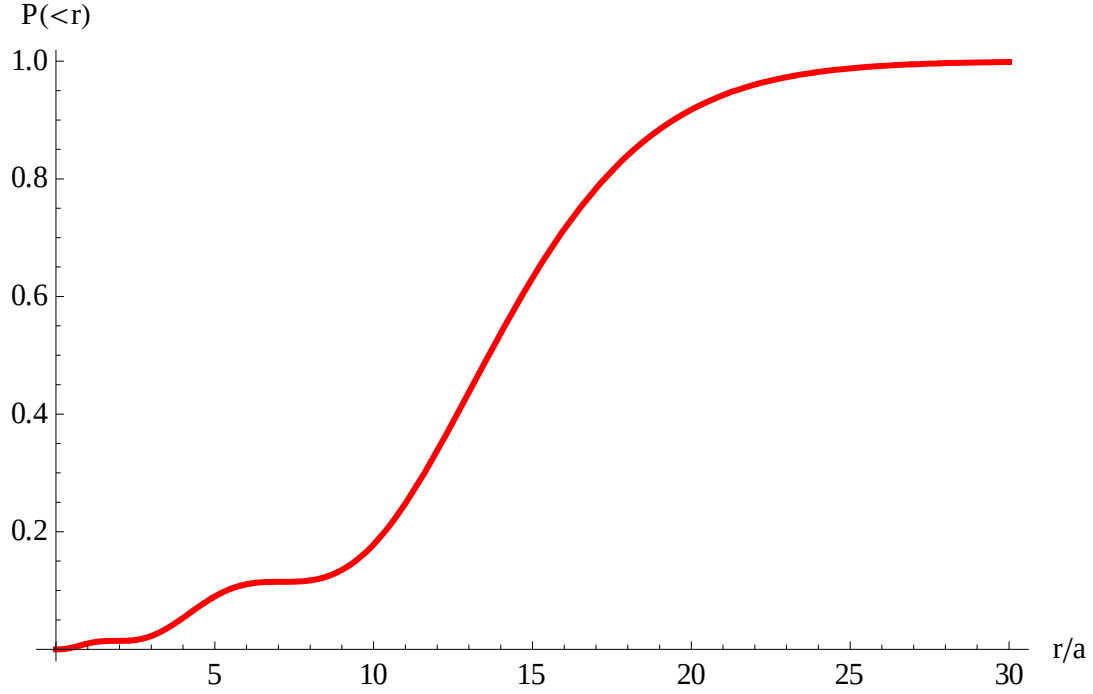


Fig. Cumulative probability density for the 3s state of hydrogen atom. $a = a_B$. $Z = 1$. $\mu = m$.

4. Radial probability distribution

The following figures show radial probability distribution $P(r) = r^2[R(r)]^2$ for a number of (n, l) states. For given (n, l) , there are number of radii where the value of $P(r)$ is zero (nodes). In general the number of such nodes is given by

$$n - l - 1.$$

The number of peaks is then given by

$$n - l.$$

If one looks carefully, at the figures, it appears that the electron will on average reside closest to the nucleus when $l = n - 1$

(a) $n = 1$ (ground state)

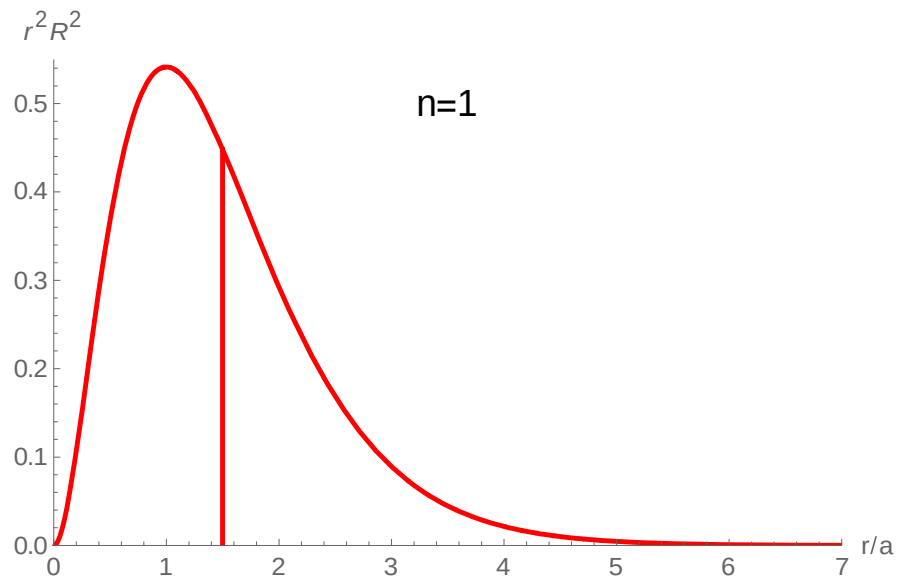


Fig. $n = 1, l = 0$ (red). The red straight line: average distance.

(b) $n = 2$

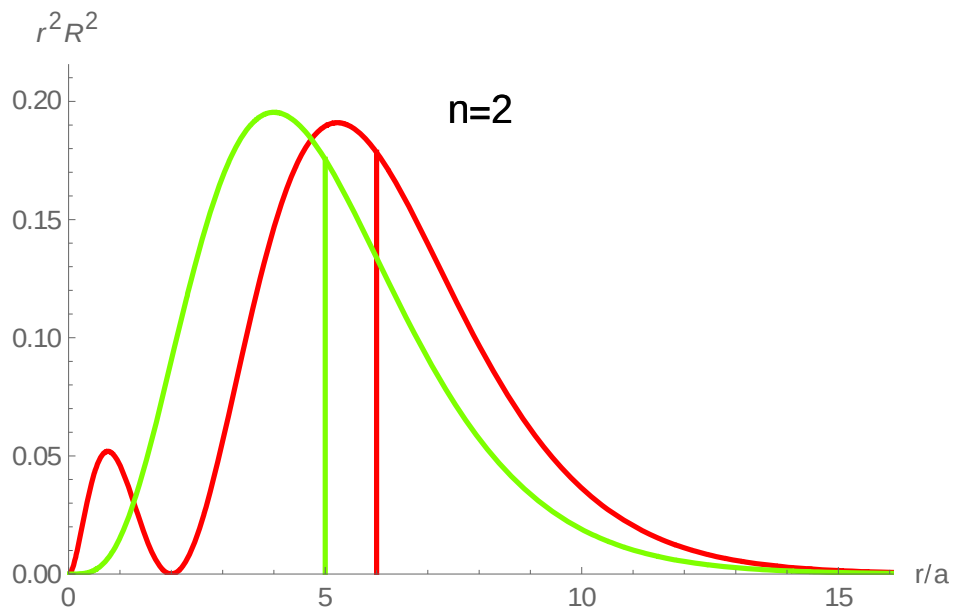


Fig. $n = 2, l = 0$ (red) and $l = 1$ (green).

(c) $n = 3$

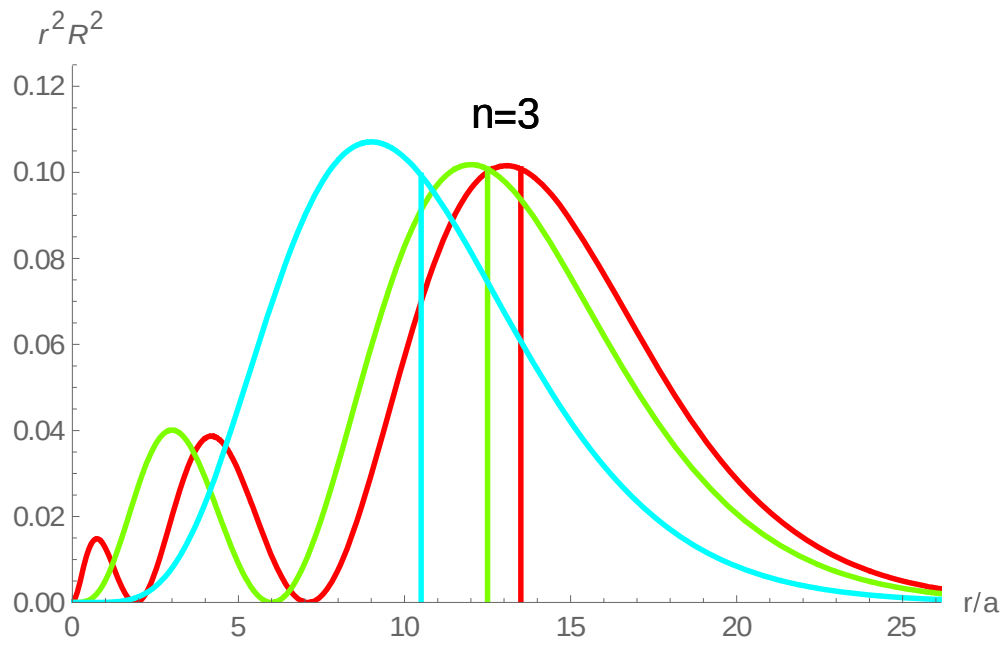


Fig. $n = 3$. $l = 0$ (red), $l = 1$ (green), and $l = 2$ (blue).

(d) $n = 4$

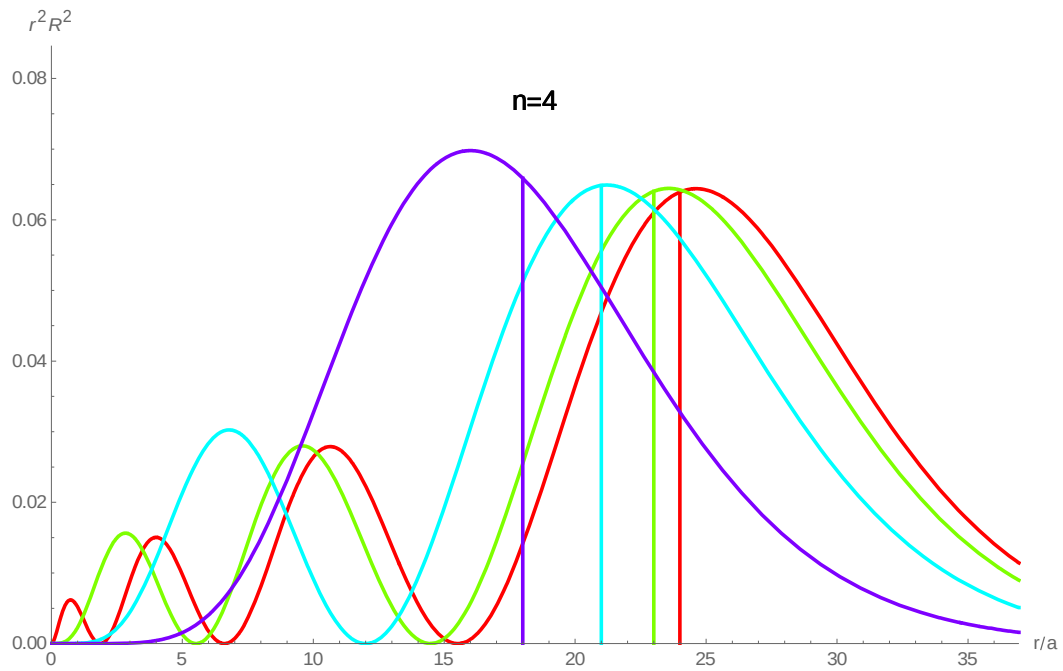


Fig. $n = 4$. $l = 0$ (red), $l = 1$ (green), $l = 2$ (blue) and $l = 3$ (purple).

REFERENCES

B.C. Reed, Quantum Mechanics (Jones and Bartlett Publishers, Sandbury MA, 2008).