> ### Robert Gilmore: Hydrogenic radial wavefunctions & overlaps

>

> R(1,0):=2*r*exp(-r);

$$R(1, 0) := 2\, r\, \mathbf{e}^{(-r)}$$

> R(2,0):=r*(1-r/2)*exp(-r/2)/sqrt(2);

$$R(2, 0) := \frac{1}{2}\, r \left(1 - \frac{1}{2}\, r \right) \mathbf{e}^{\left(-\frac{1}{2}r \right)} \sqrt{2}$$

> R(2,1):=r^2*exp(-r/2)/(2*sqrt(6));

$$R(2, 1) := \frac{1}{12}\, r^2\, \mathbf{e}^{\left(-\frac{1}{2}r \right)} \sqrt{6}$$

> R(3,0):=2*r*(1-(2/3)*r+(2/27)*r^2)*exp(-r/3)/(3*sqrt(3));

$$R(3, 0) := \frac{2}{9}\, r \left(1 - \frac{2}{3}\, r + \frac{2}{27}\, r^2 \right) \mathbf{e}^{\left(-\frac{1}{3}r \right)} \sqrt{3}$$

> R(3,1):=8/(27*sqrt(6))*r^2*(1-r/6)*exp(-r/3);

$$R(3, 1) := \frac{4}{81}\, \sqrt{6}\, r^2 \left(1 - \frac{1}{6}\, r \right) \mathbf{e}^{\left(-\frac{1}{3}r \right)}$$

> R(3,2):=4/(81*sqrt(30))*r^3*exp(-r/3);R(4,0):=(r/4)*(1-3/4*r+1/8*r^2-1/1
  92*r^3)*exp(-r/4);R(4,1):=(1/16)*sqrt(5/3)*r^2*(1-r/4+r^2/80)*exp(-r/4);
  R(4,2):=(1/64)*(1/sqrt(5))*r^3*(1-r/12)*exp(-r/4);R(4,3):=(1/768)*(1/sqr
  t(35))*r^4*exp(-r/4);

$$R(3, 2) := \frac{2}{1215}\, \sqrt{30}\, r^3\, \mathbf{e}^{\left(-\frac{1}{3}r \right)}$$

$$R(4, 0) := \frac{1}{4}\, r \left(1 - \frac{3}{4}\, r + \frac{1}{8}\, r^2 - \frac{1}{192}\, r^3 \right) \mathbf{e}^{\left(-\frac{1}{4}r \right)}$$

$$R(4, 1) := \frac{1}{48}\, \sqrt{15}\, r^2 \left(1 - \frac{1}{4}\, r + \frac{1}{80}\, r^2 \right) \mathbf{e}^{\left(-\frac{1}{4}r \right)}$$

$$R(4, 2) := \frac{1}{320}\, \sqrt{5}\, r^3 \left(1 - \frac{1}{12}\, r \right) \mathbf{e}^{\left(-\frac{1}{4}r \right)}$$

$$R(4, 3) := \frac{1}{26880} \sqrt{35}\, r^4\, e^{\left(-\frac{1}{4} r\right)}$$

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> for n from 1 to 4 do for l from 0 to n-1 do
  over(n,l):=int(R(n,l)^2,r=0..infinity):print(n,l,over(n,l)):od:od:
```

$$1, 0, 1$$
$$2, 0, 1$$
$$2, 1, 1$$
$$3, 0, 1$$
$$3, 1, 1$$
$$3, 2, 1$$
$$4, 0, 1$$
$$4, 1, 1$$
$$4, 2, 1$$
$$4, 3, 1$$

```
> for n from 1 to 4 do for l from 0 to n-1 do
  over(n,l):=int(R(n,l)^2*r,r=0..infinity):print(n,l,over(n,l)):od:od:
```

$$1, 0, \frac{3}{2}$$
$$2, 0, 6$$
$$2, 1, 5$$
$$3, 0, \frac{27}{2}$$
$$3, 1, \frac{25}{2}$$
$$3, 2, \frac{21}{2}$$
$$4, 0, 24$$
$$4, 1, 23$$
$$4, 2, 21$$
$$4, 3, 18$$

```
> for n from 1 to 4 do for l from 0 to n-1 do
  over(n,l):=int(R(n,l)^2*r^2,r=0..infinity):print(n,l,over(n,l)):od:od:
```

$$1, 0, 3$$
$$2, 0, 42$$
$$2, 1, 30$$
$$3, 0, 207$$
$$3, 1, 180$$
$$3, 2, 126$$
$$4, 0, 648$$

$$4, 1, 600$$
$$4, 2, 504$$
$$4, 3, 360$$

```
> for n from 1 to 4 do for l from 1 to n-1 do
  over(n,l):=int(R(n,l)*R(n,l-1)*1,r=0..infinity):print(n,l,over(n,l)):od:
  od:
```

$$2, 1, -\frac{1}{2}\sqrt{3}$$

$$3, 1, -\frac{2}{3}\sqrt{2}$$

$$3, 2, -\frac{1}{3}\sqrt{5}$$

$$4, 1, -\frac{1}{4}\sqrt{15}$$

$$4, 2, -\frac{1}{2}\sqrt{3}$$

$$4, 3, -\frac{1}{4}\sqrt{7}$$

```
> for n from 1 to 4 do for l from 1 to n-1 do
  over(n,l):=int(R(n,l)*R(n,l-1)*r,r=0..infinity):print(n,l,over(n,l)):od:
  od:
```

$$2, 1, -3\sqrt{3}$$
$$3, 1, -9\sqrt{2}$$
$$3, 2, -\frac{9}{2}\sqrt{5}$$
$$4, 1, -6\sqrt{15}$$
$$4, 2, -12\sqrt{3}$$
$$4, 3, -6\sqrt{7}$$

```
> for n from 1 to 4 do for l from 0 to n-1 do
  over(n,l):=int(R(n,l)*R(n,l)*r^2,r=0..infinity):print(n,l,over(n,l)):od:
  od:
```

$$1, 0, 3$$
$$2, 0, 42$$
$$2, 1, 30$$
$$3, 0, 207$$
$$3, 1, 180$$
$$3, 2, 126$$
$$4, 0, 648$$
$$4, 1, 600$$
$$4, 2, 504$$

$$4, 3, 360$$

```
> for n from 1 to 4 do for l from 2 to n-1 do
  over(n,l):=int(R(n,l)*R(n,l-2)*r^2,r=0..infinity):print(n,l,over(n,l)):o
  d:od:
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$$3, 2, 45 \sqrt{10}$$
$$4, 2, 240 \sqrt{5}$$
$$4, 3, 80 \sqrt{7} \sqrt{3}$$

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