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> ###  Prof.R. Gilmore  Quantum Mechanics 1:
> ###  Constructs the normalized hydrogen radial wavefunctions
> ###  Under (int(RX(n,l,r)*R(n,l,r)*r^2,r=0..infinity)=1
> ###  Computes energy shifts due to finite nuclear size.
>
>
>
> restart;
> with(orthopoly);    ###  calls in useful orthog polys, like the Laguerres
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$$[G, H, L, P, T, U]$$

```
> L(5,x);             ###  for example, it works
```

$$1 - 5\,x + 5\,x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5$$

```
> g(5,0,x):=L(5,x);   ###  begins process for computing Associated Laguerrs
  polys
```

$$g(5, 0, x) := 1 - 5\,x + 5\,x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5$$

```
> for i from 1 to 7 do
  g(5,i,x):=diff(g(5,i-1,x),x):print(5,i-1,g(5,i-1,x)):od:    #(it works)
```

$$5, 0, 1 - 5\,x + 5\,x^2 - \frac{5}{3}x^3 + \frac{5}{24}x^4 - \frac{1}{120}x^5$$

$$5, 1, -5 + 10\,x - 5\,x^2 + \frac{5}{6}x^3 - \frac{1}{24}x^4$$

$$5, 2, 10 - 10\,x + \frac{5}{2}x^2 - \frac{1}{6}x^3$$

$$5, 3, -10 + 5\,x - \frac{1}{2}x^2$$

$$5, 4, 5 - x$$

$$5, 5, -1$$

$$5, 6, 0$$

```
> for j from 0 to 12 do g(j,0,x):=L(j,x);for i from 1 to j+2 do
  g(j,i,x):=diff(g(j,i-1,x),x):od:od:##  Lots of assoc lag.
> for n from 1 to 5 do for l from 0 to n-1 do R(n,l,x):=
  g(n+l,2*l+1,x)*exp(-x/2)*(x)^l:RR(n,l,r):=subs(x=2*r/n,%):N(n,l):=int(r^
  2*RR(n,l,r)^2,r=0..infinity):RX(n,l,r):=RR(n,l,r)/sqrt(N(n,l));print(n,l
  ,RX(n,l,r)):od:od:   ### constructs normalized hydrogenic radial
  wavefunctions
```

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

$$2,\ 0,\ \frac{1}{4}(-2+r)\,\mathbf{e}^{\left(-\frac{1}{2}r\right)}\sqrt{2}$$

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

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

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

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

$$4,\ 0,\ \frac{1}{16}\left(-4+3r-\frac{1}{2}r^2+\frac{1}{48}r^3\right)\mathbf{e}^{\left(-\frac{1}{4}r\right)}$$

$$4,\ 1,\ \frac{1}{480}\left(-10+\frac{5}{2}r-\frac{1}{8}r^2\right)\mathbf{e}^{\left(-\frac{1}{4}r\right)}r\sqrt{15}$$

$$4,\ 2,\ \frac{1}{1920}\left(-6+\frac{1}{2}r\right)\mathbf{e}^{\left(-\frac{1}{4}r\right)}r^2\sqrt{5}$$

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

$$5,\ 0,\ \frac{2}{125}\left(-5+4r-\frac{4}{5}r^2+\frac{4}{75}r^3-\frac{2}{1875}r^4\right)\mathbf{e}^{\left(-\frac{1}{5}r\right)}\sqrt{5}$$

$$5,\ 1,\ \frac{1}{1875}\left(-20+6r-\frac{12}{25}r^2+\frac{4}{375}r^3\right)\mathbf{e}^{\left(-\frac{1}{5}r\right)}r\sqrt{30}$$

$$5,\ 2,\ \frac{2}{65625}\left(-21+\frac{14}{5}r-\frac{2}{25}r^2\right)\mathbf{e}^{\left(-\frac{1}{5}r\right)}r^2\sqrt{70}$$

$$5,\ 3,\ \frac{1}{328125}\left(-8+\frac{2}{5}r\right)\mathbf{e}^{\left(-\frac{1}{5}r\right)}\ r^3\sqrt{70}$$

$$5,\ 4,\ -\frac{2}{4921875}\mathbf{e}^{\left(-\frac{1}{5}r\right)}\ r^4\sqrt{70}$$

```
> ### for n from 1 to 5 do for l from 0 to n-1 do
  print(n,l,RX(n,l,r)):od:od:
```

```
> for n from 1 to 5 do for l from 1 to n-1 do
  over(n,l):=int(RX(n,l,r)*RX(n,l-1,r)*r*r^2,r=0..infinity):print(n,l,over
  (n,l)):od:od:
```

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

$$3,\ 1,\ -9\sqrt{2}$$

$$3,\ 2,\ -\frac{9}{2}\sqrt{5}$$

$$4,\ 1,\ -6\sqrt{15}$$

$$4,\ 2,\ -12\sqrt{3}$$

$$4,\ 3,\ -6\sqrt{7}$$

$$5,\ 1,\ -15\sqrt{6}$$

$$5,\ 2,\ -\frac{15}{2}\sqrt{7}\sqrt{3}$$

$$5,\ 3,\ -30$$

$$5,\ 4,\ \frac{-45}{2}$$

```
> for n from 1 to 5 do for l from 0 to n-1 do
  over(n,l):=int(RX(n,l,r)*RX(n,l,r)*r^2*r^2,r=0..infinity):print(n,l,over
  (n,l)):od:od:
```

$$1,\ 0,\ 3$$

$$2,\ 0,\ 42$$

$$2,\ 1,\ 30$$

$$3,\ 0,\ 207$$

$$3,\ 1,\ 180$$

$$3,\ 2,\ 126$$

$$4,\ 0,\ 648$$

$$4,\ 1,\ 600$$

$$4,\ 2,\ 504$$

$$4,\ 3,\ 360$$

$$5,\ 0,\ 1575$$

$$5,\ 1,\ 1500$$

$$5, 2, 1350$$

$$5, 3, 1125$$

$$5, 4, 825$$

```
> for n from 1 to 5 do for l from 2 to n-1 do
  over(n,l):=int(RX(n,l,r)*RX(n,l-2,r)*r^2*r^2,r=0..infinity):print(n,l,ov
  er(n,l)):od:od:
```

$$3, 2, 45\sqrt{10}$$

$$4, 2, 240\sqrt{5}$$

$$4, 3, 80\sqrt{7}\sqrt{3}$$

$$5, 2, 375\sqrt{14}$$

$$5, 3, 250\sqrt{7}\sqrt{3}$$

$$5, 4, 750$$

```
> pert1:=-3/(2*K)+(r/K)^2/(2*K)+1/r;
```

$$pert1 := -\frac{3}{2K} + \frac{r^2}{2K^3} + \frac{1}{r}$$

```
> pert2:=-1/K+1/r;
```

$$pert2 := -\frac{1}{K} + \frac{1}{r}$$

```
> int(RX(1,0,r)^2*r^2*pert1,r=0..K);taylor(%,K=0,10);
```

$$\frac{3 - 3K^2 + 2K^3 - 3\mathbf{e}^{(-2K)} - 3\mathbf{e}^{(-2K)}K^2 - 6\mathbf{e}^{(-2K)}K}{2K^3}$$

$$\frac{2}{5}K^2 - \frac{1}{3}K^3 + \frac{6}{35}K^4 - \frac{1}{15}K^5 + \frac{4}{189}K^6 + O(K^7)$$

```
> int(RX(1,0,r)^2*r^2*pert2,r=0..K);taylor(%,K=0,10);
```

$$\frac{-1 + K + \mathbf{e}^{(-2K)} + \mathbf{e}^{(-2K)}K}{K}$$

$$\frac{2}{3}K^2 - \frac{2}{3}K^3 + \frac{2}{5}K^4 - \frac{8}{45}K^5 + \frac{4}{63}K^6 - \frac{2}{105}K^7 + \frac{2}{405}K^8 + O(K^9)$$

```
> for n from 1 to 5 do for l from 0 to n-1 do z:= int(RX(n,l,r)^2*r^2*pert1
  ,r=0..K);corr1(n,l):=taylor(%,K=0,8+2*l):print(n,l,corr1(n,l)):od:od:
```

$$1, 0, \frac{2}{5}K^2 - \frac{1}{3}K^3 + \frac{6}{35}K^4 + O(K^5)$$

$$2, 0, \frac{1}{20}K^2 - \frac{1}{24}K^3 + \frac{3}{160}K^4 + O(K^5)$$

$$2, 1, \frac{1}{1120}K^4 - \frac{1}{1920}K^5 + \frac{1}{6048}K^6 + O(K^7)$$

$$3,\ 0,\ \frac{2}{135}K^2 - \frac{1}{81}K^3 + \frac{46}{8505}K^4 + O(K^5)$$

$$3,\ 1,\ \frac{8}{25515}K^4 - \frac{2}{10935}K^5 + \frac{68}{1240029}K^6 + O(K^7)$$

$$3,\ 2,\ \frac{4}{6200145}K^6 - \frac{1}{3444525}K^7 + \frac{2}{29229255}K^8 + O(K^9)$$

$$4,\ 0,\ \frac{1}{160}K^2 - \frac{1}{192}K^3 + \frac{81}{35840}K^4 + O(K^5)$$

$$4,\ 1,\ \frac{1}{7168}K^4 - \frac{1}{12288}K^5 + \frac{37}{1548288}K^6 + O(K^7)$$

$$4,\ 2,\ \frac{1}{2580480}K^6 - \frac{1}{5734400}K^7 + \frac{31}{778567680}K^8 + O(K^9)$$

$$4,\ 3,\ \frac{1}{5449973760}K^8 - \frac{1}{14863564800}K^9 + \frac{1}{78721843200}K^{10} + O(K^{11})$$

$$5,\ 0,\ \frac{2}{625}K^2 - \frac{1}{375}K^3 + \frac{18}{15625}K^4 + O(K^5)$$

$$5,\ 1,\ \frac{8}{109375}K^4 - \frac{2}{46875}K^5 + \frac{916}{73828125}K^6 + O(K^7)$$

$$5,\ 2,\ \frac{4}{17578125}K^6 - \frac{1}{9765625}K^7 + \frac{334}{14501953125}K^8 + O(K^9)$$

$$5,\ 3,\ \frac{16}{101513671875}K^8 - \frac{8}{138427734375}K^9 + \frac{28}{2618408203125}K^{10} + O(K^{11})$$

$$5,\ 4,\ \frac{4}{164959716796875}K^{10} - \frac{2}{266473388671875}K^{11} + \frac{4}{3374176025390625}K^{12} + O(K^{13})$$

```
> for n from 1 to 5 do for l from 0 to n-1 do
  z:=int(RX(n,l,r)^2*r^2*pert2,r=0..K);corr1(n,l):=taylor(%,K=0,6+2*l):pri
  nt(n,l,corr1(n,l)):od:od:
```

$$1,\ 0,\ \frac{2}{3}K^2 - \frac{2}{3}K^3 + \frac{2}{5}K^4 + O(K^5)$$

$$2,\ 0,\ \frac{1}{12}K^2 - \frac{1}{12}K^3 + \frac{7}{160}K^4 + O(K^5)$$

$$2,\ 1,\ \frac{1}{480}K^4 - \frac{1}{720}K^5 + \frac{1}{2016}K^6 + O(K^7)$$

$$3,\ 0,\ \frac{2}{81}K^2 - \frac{2}{81}K^3 + \frac{46}{3645}K^4 + O(K^5)$$

$$3,\ 1,\ \frac{8}{10935}K^4 - \frac{16}{32805}K^5 + \frac{68}{413343}K^6 + O(K^7)$$

$$3,\ 2,\ \frac{4}{2066715}K^6 - \frac{2}{2066715}K^7 + \frac{2}{7971615}K^8 + O(K^9)$$

$$4,\ 0,\ \frac{1}{96}K^2 - \frac{1}{96}K^3 + \frac{27}{5120}K^4 + O(K^5)$$

$$4,\ 1,\ \frac{1}{3072}K^4 - \frac{1}{4608}K^5 + \frac{37}{516096}K^6 + O(K^7)$$

$$4,\ 2,\ \frac{1}{860160}K^6 - \frac{1}{1720320}K^7 + \frac{31}{212336640}K^8 + O(K^9)$$

$$4,\ 3,\ \frac{1}{1486356480}K^8 - \frac{1}{3715891200}K^9 + \frac{1}{18166579200}K^{10} + O(K^{11})$$

$$5,\ 0,\ \frac{2}{375}K^2 - \frac{2}{375}K^3 + \frac{42}{15625}K^4 + O(K^5)$$

$$5,\ 1,\ \frac{8}{46875}K^4 - \frac{16}{140625}K^5 + \frac{916}{24609375}K^6 + O(K^7)$$

$$5,\ 2,\ \frac{4}{5859375}K^6 - \frac{2}{5859375}K^7 + \frac{334}{3955078125}K^8 + O(K^9)$$

$$5,\ 3,\ \frac{16}{27685546875}K^8 - \frac{32}{138427734375}K^9 + \frac{28}{604248046875}K^{10} + O(K^{11})$$

$$5,\ 4,\ \frac{4}{38067626953125}K^{10} - \frac{4}{114202880859375}K^{11} + \frac{4}{674835205078125}K^{12} + O(K^{13})$$

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