Quantum Mech. Applications 2.Hidrogen Atom in spherical coordinates

Introduction

```
ClearAll["Global`*"]
Off[General::spell, General::spell1]
```

Using package

```
Needs["Graphics`ParametricPlot3D`"];
```

Solution

```
Clear["Global`*"];
```

■ Step1 The Radial equation is

eq1 =

$$0 == \frac{2\, m\, R(r)\, (\text{En} - V(r))\, r^2}{\hbar^2} + R''(r)\, r^2 + 2\, R'(r)\, r - \ell\, (\ell + 1)\, R(r) \text{ /. V[r]} \to -\frac{e^2}{4\, \pi\, r\, \epsilon 0} \text{ /. En} \to -\text{Wn}$$

$$0 == -\ell\, (1 + \ell)\, \text{R[r]} + \frac{2\, m\, r^2 \left(-\text{Wn} + \frac{e^2}{4\, \pi\, r\, \epsilon 0}\right) \text{R[r]}}{\hbar^2} + 2\, r\, \text{R}'[r] + r^2\, \text{R}''[r]$$

■ Step2 Searching for the solutions of the Radial equation

eq2=DSolve[eq1,{R[r]},r][[1]]

$$\left\{R[r]\to e^{-\frac{\sqrt{2}\sqrt{m}\,r\sqrt{Wn}}{\hbar}+\ell\,\mathrm{Log}[r]}\,C[1]\,\mathrm{HypergeometricU}\left[-\frac{\sqrt{2}\,e^2\sqrt{m}-8\pi\sqrt{Wn}\,\epsilon0\,\hbar-8\pi\sqrt{Wn}\,\ell\,\epsilon0\,\hbar}{8\pi\sqrt{Wn}\,\epsilon0\,\hbar},\ 2+2\ell,\ \frac{2\sqrt{2}\sqrt{m}\,r\sqrt{Wn}}{\hbar}\right]+e^{-\frac{\sqrt{2}\sqrt{m}\,r\sqrt{Wn}}{\hbar}+\ell\,\mathrm{Log}[r]}\,C[2]\,\mathrm{LaguerreL}\left[\frac{\sqrt{2}\,e^2\sqrt{m}-8\pi\sqrt{Wn}\,\epsilon0\,\hbar-8\pi\sqrt{Wn}\,\ell\,\epsilon0\,\hbar}{8\pi\sqrt{Wn}\,\epsilon0\,\hbar},\ 1+2\ell,\ \frac{2\sqrt{2}\sqrt{m}\,r\sqrt{Wn}}{\hbar}\right]\right\}$$

substitutions =

$$\left\{m\to\frac{4\pi\epsilon0\,\hbar^2}{a0\,e^2},\ Wn\to\frac{e^4\,m}{32\,n^2\,\pi^2\,\epsilon0^2\,\hbar^2}\right\};$$

```
eq3 = eq2 //. substitutions // PowerExpand //
    Simplify
```

$$\left\{R[r] \to e^{-\frac{r}{a0\, n}}\, r^{\ell} \left(C[1]\, \text{HypergeometricU}\left[1-n+\ell,\, 2+2\,\ell,\, \frac{2\,r}{a0\,n}\right] + C[2]\, \text{LaguerreL}\left[-1+n-\ell,\, 1+2\,\ell,\, \frac{2\,r}{a0\,n}\right]\right)\right\}$$

```
eq4 = eq3 /. {C[1] → 0 }
```

$$\left\{R[r] \to e^{-\frac{r}{a0\, n}}\, r^{\ell}\, C[2]\, \text{LaguerreL}\left[-1+n-\ell,\, 1+2\,\ell,\, \frac{2\,r}{a0\,n}\right]\right\}$$

$$\mathbf{rNorm} = 2^{\ell+1}\left(\frac{1}{a0\, n}\right)^{\ell} \sqrt{\frac{(n-\ell-1)!}{a0^{3}\, n^{4}\, (n+\ell)!}}\;;$$

```
rwave[n_, ℓ_, r_] =
  R[r] /. eq4[[1]] /. C[2] → rNorm // PowerExpand //
    Simplify
```

$$\frac{1}{\sqrt{(n+\ell)!}}\, 2^{1+\ell}\, a0^{-\frac{3}{2}-\ell}\, e^{-\frac{r}{a0\,n}}\, n^{-2-\ell}\, r^{\ell} \sqrt{(-1+n-\ell)!}\, \text{LaguerreL}\left[-1+n-\ell,\, 1+2\,\ell,\, \frac{2\,r}{a0\,n}\right]$$

```
Integrate[
  r^2
    { rwave[1, 0, r], rwave[2, 0, r],
         rwave[2, 1, r]}^2, {r, 0, ∞},
  Assumptions → {Re[a0] > 0}]
```

```
{1, 1, 1}
```

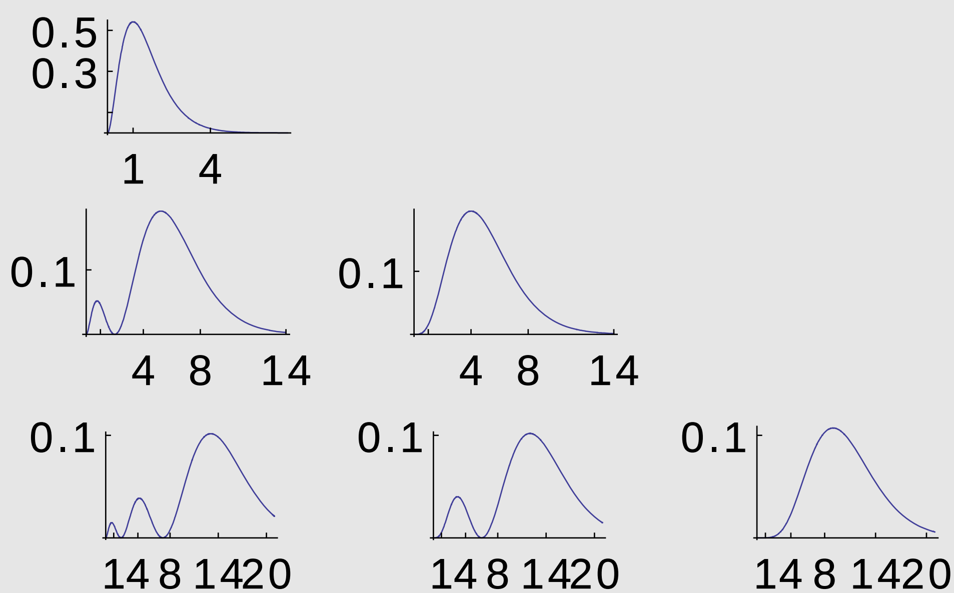
■ Step 3 Representing the results (the form of the wave functions for n=1,2,3)

```
eq5 =
  Table[rwave[n, ℓ, r], {n, 1, 3}, {ℓ, 0, n − 1}] //
    TableForm[#,
       TableHeadings →
         {{"n=1", "n=2", "n=3"},
           {"ℓ=0", "ℓ=1", "ℓ=2"}}] &
```

	$\ell=0$	$\ell=1$	$\ell=2$
n=1	$\frac{2\,e^{-\frac{r}{a0}}}{a0^{3/2}}$		
n=2	$\frac{e^{-\frac{r}{2\,a0}}\left(2-\frac{r}{a0}\right)}{2\sqrt{2}\,a0^{3/2}}$	$\frac{e^{-\frac{r}{2\,a0}}\,r}{2\sqrt{6}\,a0^{5/2}}$	
n=3	$\frac{2\,e^{-\frac{r}{3\,a0}}\left(27\,a0^2-18\,a0\,r+2\,r^2\right)}{81\sqrt{3}\,a0^{7/2}}$	$\frac{\sqrt{\frac{2}{3}}\,e^{-\frac{r}{3\,a0}}\,r\left(4-\frac{2\,r}{3\,a0}\right)}{27\,a0^{5/2}}$	$\frac{2\sqrt{\frac{2}{15}}}{81}$

```
plot[n_, ℓ_, rmax_] :=
    Plot[r^2 rwave[n, ℓ, r]^2 /. a0 → 1 // Evaluate,
      {r, 0.01, rmax},
      Ticks → {{1, 4, 8, 14, 20}, {0.1, 0.3, 0.5}},
      DisplayFunction → Identity];
```

```
Show[GraphicsGrid[
    Table[plot[n, ℓ, n 7], {n, 1, 3}, {ℓ, 0, n – 1}]]]
```



■ Step 4 Representing the spherical function in 3D

```
plot[ℓ_, m_] :=
    SphericalPlot3D[
      SphericalHarmonicY[ℓ, m, θ, ϕ] // Abs //
        Evaluate,
      {θ, 0, π}, {ϕ, 0, 2 π},
      Boxed → False,
      Axes → False,
      DisplayFunction → Identity];
```

```
pt1 = Table[plot[ℓ, m], {ℓ, 0, 2}, {m, -ℓ, ℓ}];
Show[GraphicsGrid[pt1]]
```