```
In[122]:= DateList[]

Out[122]= {2009, 11, 12, 17, 43, 49.674079}
```

Orbital 1s

1s radial wave function

$$ps1[r\_] := 4 \left(\frac{Z}{a}\right)^3 \text{Exp}\left[-\frac{2 Z r}{a}\right] r^2$$

Check normalization

$$\text{Integrate}\left[ps1[r], \{r, 0, \infty\}, \text{Assumptions} \to \text{Re}\left[\frac{Z}{a}\right] > 0\right]$$

$$1$$

Calculate the average R

$$\text{Integrate}\left[r\, ps1[r], \{r, 0, \infty\}, \text{Assumptions} \to \text{Re}\left[\frac{Z}{a}\right] > 0\right]$$

$$\frac{3 a}{2 Z}$$

Average 1/R

$$\text{Integrate}\left[\frac{ps1[r]}{r}, \{r, 0, \infty\}, \text{Assumptions} \to \text{Re}\left[\frac{Z}{a}\right] > 0\right]$$

$$\frac{Z}{a}$$

Average R^2

$$\text{Integrate}\left[r^2\, ps1[r], \{r, 0, \infty\}, \text{Assumptions} \to \text{Re}\left[\frac{Z}{a}\right] > 0\right]$$

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

Average R^n

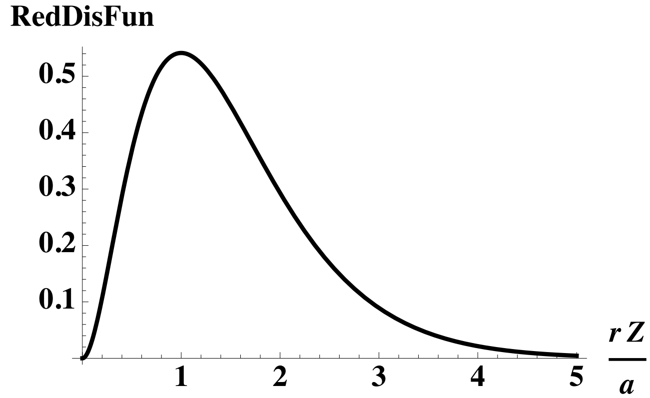
$$\text{Integrate}\left[r^n\, ps1[r], \{r, 0, \infty\}, \text{Assumptions} \to \left\{\text{Re}\left[\frac{Z}{a}\right] > 0, \text{Re}[n] > 0\right\}\right]$$

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

Plot the probability as a function of R

In[46]:=
```
Plot[ps1[r] /. {Z → 1, a → 1}, {r, 0, 5}, BaseStyle → {Bold, 14},
 PlotStyle → {Thick, Black}, AxesLabel → {r Z / a, RedDisFun}]
```

Out[46]=



Determine the max of the probability

```
d1 = D[ps1[r], {r}]
```

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

Solve for Rmax

```
rmax = Solve[d1 == 0, r]
```

$$\left\{\{r \to 0\},\ \left\{r \to \frac{a}{Z}\right\}\right\}$$

```
rmax[[1]]
rmax[[2]]
```

$\{r \to 0\}$

$\left\{r \to \frac{a}{Z}\right\}$

```
ps1[a / Z] (a / Z) // N
```

0.541341

Probability from zero to a/Z

```
Integrate[ps1[r], {r, 0, a / Z}, Assumptions → Re[Z/a] > 0] // N
```

0.323324

probability from zero to Raverage

```
Integrate[ps1[r], {r, 0, 3 a / (2 Z)}, Assumptions → Re[Z/a] > 0] // N
```

0.57681

Probability from zero to x a/z - distance in units of a/Z

```
prob[x_] = Integrate[ps1[r], {r, 0, x a / Z}, Assumptions → Re[Z/a] > 0] // N
```

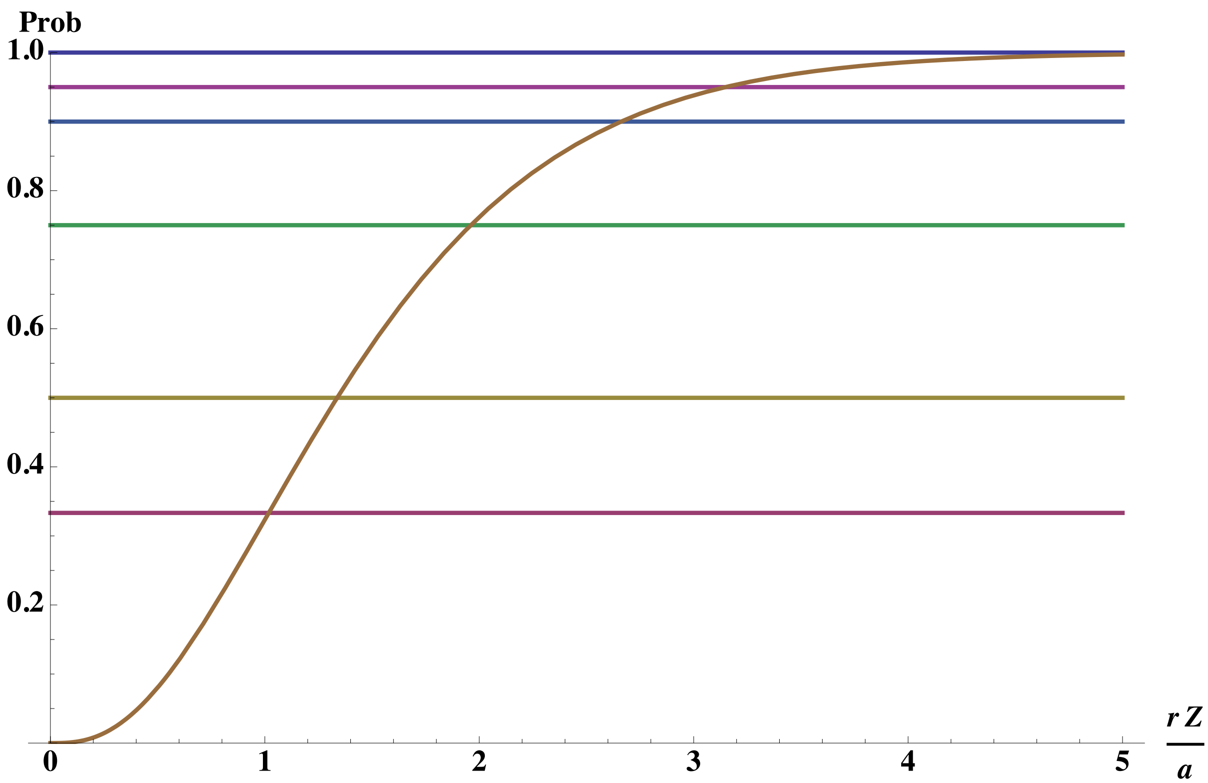
$1. + 2.71828^{-2. x} (-1. - 2. x (1. + x))$

```
NSolve[prob[x] == .90, x]
```

Solve::tdep :
The equations appear to involve the variables to be solved for in an essentially non-algebraic way. ≫

$\text{NSolve}[1. + 2.71828^{-2. x} (-1. - 2. x (1. + x)) == 0.9, x]$

```
Plot[Evaluate[{1, 1 / 3, 1 / 2, 3 / 4, .9, .95, prob[x]}], {x, 0, 5}, PlotRange → {0, 1},
 PlotStyle → {Thick}, BaseStyle → {Bold, 14}, AxesLabel → {r Z / a, Prob}]
```



Orbital 3s

Consider the 3s orbital

In[71]:= $\text{wf3s}[r\_, \text{theta}\_, \text{phi}\_] := \frac{\left(\frac{Z}{a}\right)^{3/2} \left(27 - \frac{18 Z r}{a} + \frac{2 Z^2 r^2}{a^2}\right) \text{Exp}\left[-\frac{Z r}{3 a}\right]}{81 \sqrt{3 \pi}}$

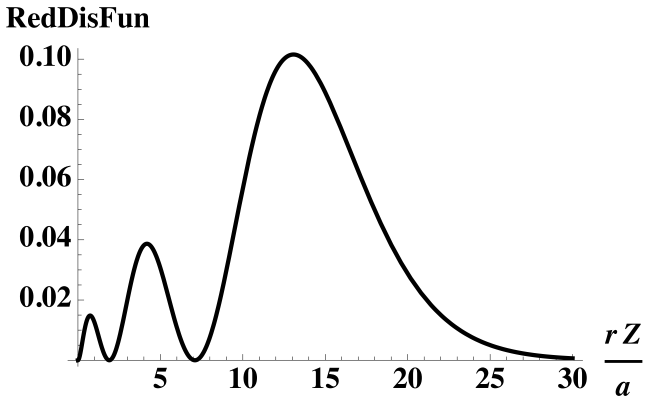
In[81]:= `prob3s[r_] := (4 π) wf3s[r, theta, phi]^2 r^2`

In[73]:= $\text{Integrate}\left[\text{prob3s}[r], \{r, 0, \infty\}, \text{Assumptions} \to \text{Re}\left[\frac{Z}{a}\right] > 0\right]$

Out[73]= 1

In[74]:=
```
Plot[prob3s[r] /. {Z → 1, a → 1}, {r, 0, 30}, BaseStyle → {Bold, 14},
 PlotStyle → {Thick, Black}, AxesLabel → {r Z / a, RedDisFun}]
```

Out[74]=

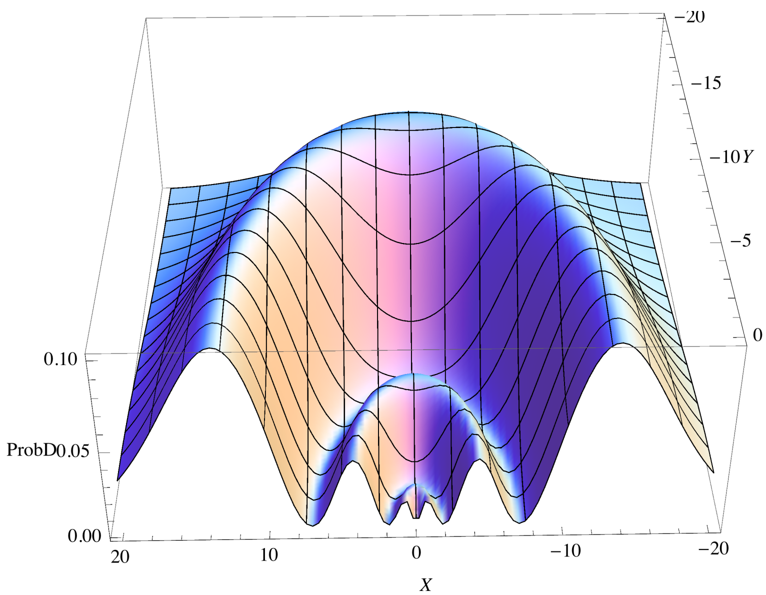


The orbital in cartesian coordinates and z=0

In[51]:=
```
p3s[x_, y_] := prob3s[Sqrt[x^2 + y^2]] /. {Z → 1, a → 1}
```

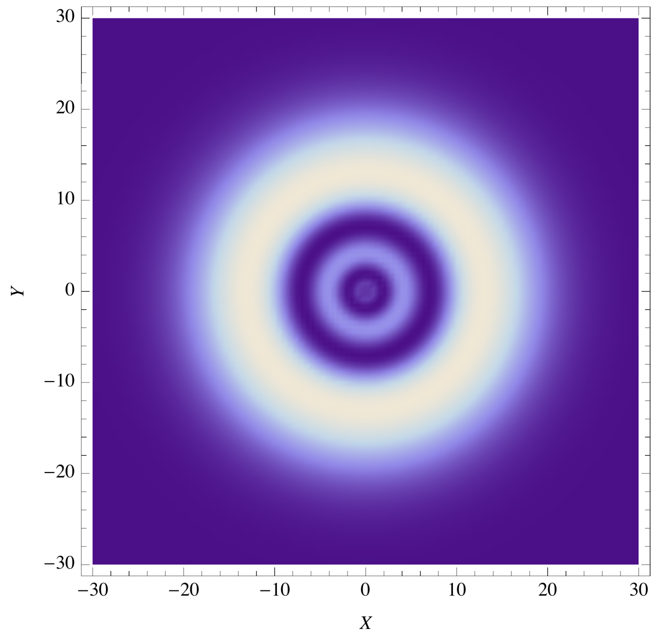
In[57]:=
```
Plot3D[p3s[x, y], {x, -20, 20}, {y, -20, 0}, PlotPoints → 100, AxesLabel → {X, Y, ProbD}]
```

Out[57]=



In[121]:=
```
DensityPlot[p3s[x, y], {x, -30, 30}, {y, -30, 30}, PlotPoints → 100, FrameLabel → {X, Y}]
```

Out[121]=



Average R

In[83]:=
```
Integrate[r prob3s[r], {r, 0, Infinity}, Assumptions → Re[Z/a] > 0]
```

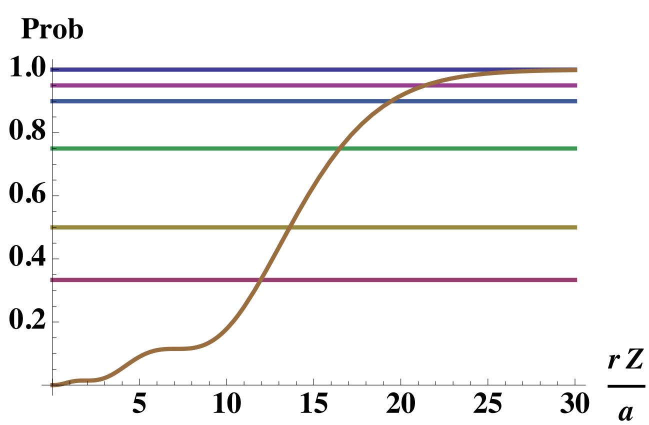
Out[83]= $\frac{27\,a}{2\,Z}$

In[84]:=
```
prob3[x_] = Integrate[prob3s[r], {r, 0, x a / Z}, Assumptions → Re[Z/a] > 0] // N
```

Out[84]= $1. + 0.000152416 \times 2.71828^{-0.666667\,x}\left(-6561. - 2.\,x\left(2187. + x\left(729. + 2.\,x^2\,(81. + 2.\,(-9. + x)\,x)\right)\right)\right)$

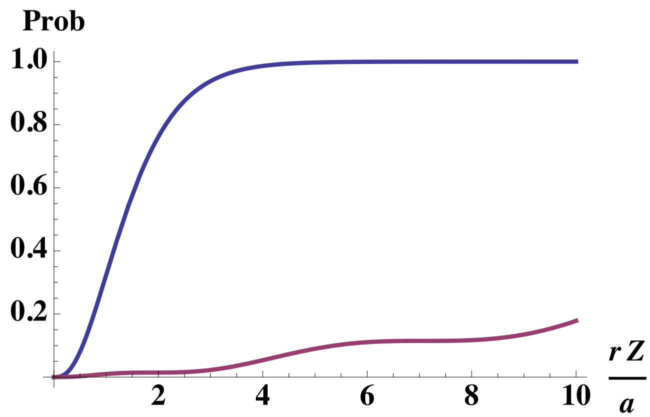
In[86]:=
```
Plot[Evaluate[{1, 1 / 3, 1 / 2, 3 / 4, .9, .95, prob3[x]}], {x, 0, 30}, PlotRange → All,
  PlotStyle → {Thick}, BaseStyle → {Bold, 14}, AxesLabel → {r Z / a, Prob}]
```

Out[86]=



In[88]:=
```
Plot[Evaluate[{prob[x], prob3[x]}], {x, 0, 10}, PlotRange → All,
  PlotStyle → {Thick}, BaseStyle → {Bold, 14}, AxesLabel → {r Z / a, Prob}]
```

Out[88]=



Orbital 3py

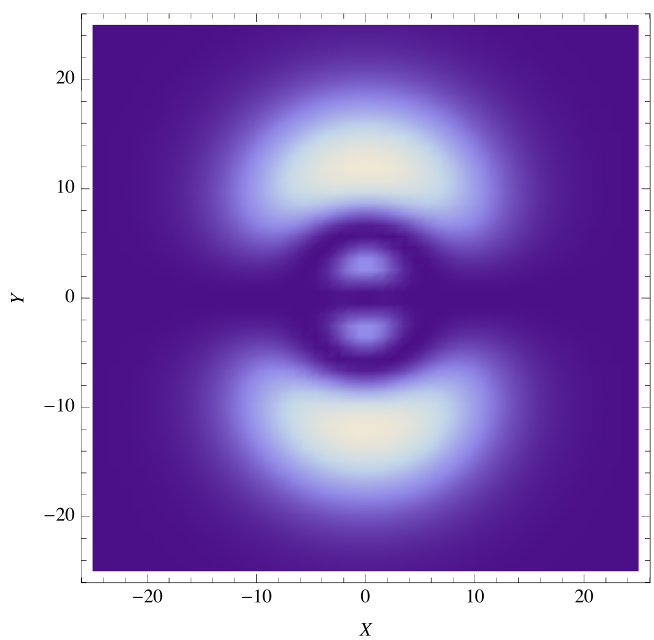
Orbital 3Py in cartesian coordinates and z=0

In[104]:=

$$pD3py[x\_, y\_] := \left(\frac{\sqrt{2}\left(\frac{Z}{a}\right)^{3/2}\left(\frac{6\,Z\sqrt{x^2+y^2}}{a} - \frac{\sqrt{x^2+y^2}^{\,2}\,Z^2}{a^2}\right)\mathrm{Exp}\left[-\frac{\sqrt{x^2+y^2}\,Z}{3\,a}\right]y}{\left(81\sqrt{\pi}\right)\sqrt{x^2+y^2}}\right)^2 \sqrt{x^2+y^2}^{\,2} \;/.\; \{Z \to 1,\ a \to 1\}$$

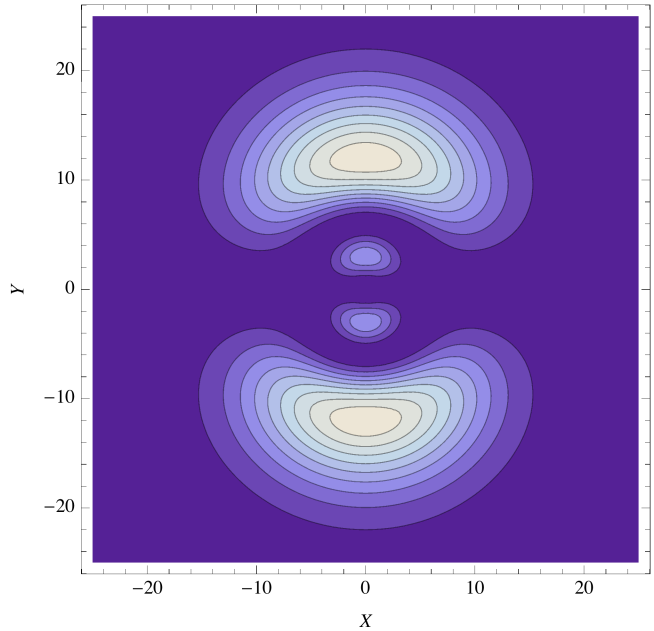
In[118]:=
```
DensityPlot[pD3py[x, y], {x, -25 , 25}, {y, -25, 25}, FrameLabel → {X, Y}, PlotPoints → 50]
```

Out[118]=



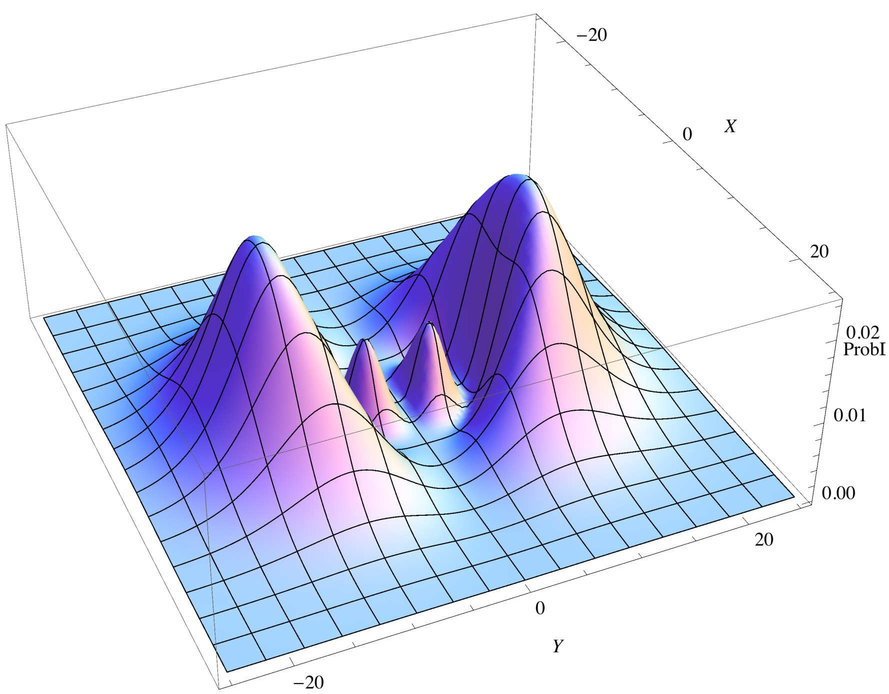
In[117]:=
```
ContourPlot[pD3py[x, y], {x, -25 , 25}, {y, -25, 25}, PlotPoints → 50, FrameLabel → {X, Y}]
```

Out[117]=



In[120]:=
```
Plot3D[pD3py[x, y], {x, -25, 25}, {y, -25, 25}, PlotPoints → 100, AxesLabel → {X, Y, ProbD}]
```

Out[120]=



Virial Theorem

$$\langle 2K \rangle = \langle \underset{\sim}{r} \cdot \nabla V \rangle$$

HO $\quad 2\langle K \rangle = \langle x \frac{\partial}{\partial x} V \rangle = 2\langle V \rangle$

$$V = \frac{1}{2} k x^2$$

$$\Rightarrow \quad \langle K \rangle = \langle V \rangle = \frac{1}{2} \langle H \rangle = \frac{1}{2} E_n$$

Hydrogen $\quad V = + \frac{K}{r}$

$$\underset{\sim}{r} \cdot \nabla V = - V$$

$$2\langle K \rangle = - \langle V \rangle$$

$$\langle K \rangle = - \frac{1}{2} \langle V \rangle$$

$$\langle K \rangle + \langle V \rangle = \langle H \rangle$$

$$-\frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle$$

$\Rightarrow$

$$\langle V \rangle = 2 \langle H \rangle = 2 E_n$$

$$\langle K \rangle = - E_n$$

Q II. Hydrogen Atom

μ — $[\mu] = M$

$\hbar$ — $[\hbar] = M L^2 T^{-2} T$

K — $[K] = M L^2 T^{-2} L^{+}$

$V = \frac{K}{r}$ $K = -\frac{Z|e|^2}{4\pi\epsilon_0}$

$$[\mu^\alpha \hbar^\beta K^\gamma] = M L^2 T^{-2}$$

$$M^\alpha M^\beta L^{2\beta} T^{-\beta} M^\gamma L^{3\gamma} T^{-2\gamma}$$

$$\alpha + \beta + \gamma = 1$$
$$2\beta + 3\gamma = 2$$

$$\beta + 2\gamma = 2$$
$$\beta = 2(1-\gamma) = 2 - 2\gamma$$
$$2\beta = 4 - 4\gamma$$

$$4 - 4\gamma + 3\gamma = 2$$

$$\boxed{\gamma = +2}$$
$$\boxed{\beta = -2}$$
$$\boxed{\alpha = 1}$$

$$E \sim \frac{\mu K^2}{\hbar^2} = \frac{\mu Z^2 |e|^4}{\hbar^2 (4\pi)^2 \epsilon_0^2} = \frac{\mu Z^2 |e|^4}{4 \hbar^2 \epsilon_0^2}$$