Allure des orbitales, en coupe, par un tracé de courbes iso-probabilité

restart

```
amplitude := proc(x :: float, z :: float, typo :: string) :: float;
 local
  r, th, aa :: float;
  r := sqrt(x^2 + z^2);
  if (r = 0.00) then th := 0.00;
  else th := arcsin(|x| / r);
  end if;
  if typo = "s3" then aa := (3·a0)^(-3/2) / sqrt(π) · (1 - 2·r/(3·a0) + 2/3·(r/(3·a0))^2) · exp(-r/(3·a0));
  elif typo = "p3x" then aa := (3·a0)^(-3/2) / sqrt(3/2·π) · (r/(3·a0)) · (2 - r/(3·a0)) · exp(-r/(3·a0)) · sin(th);
  elif typo = "p3z" then aa := (3·a0)^(-3/2) / sqrt(3/2·π) · (r/(3·a0)) · (2 - r/(3·a0)) · exp(-r/(3·a0)) · cos(th);
  elif typo = "d3z2" then aa := (3·a0)^(-3/2) / sqrt(6·π) · (r/(3·a0))^2 · exp(-r/(3·a0)) · (3·cos^2(th) - 1);
  elif typo = "d3zx" then aa := (3·a0)^(-3/2) / sqrt(6·π) · (r/(3·a0))^2 · exp(-r/(3·a0)) · sin(2·th);
  else aa := 0.00;
 end if;
  aa := evalf(aa);
  return(aa);
end proc: #amplitude

AmpliMax := proc(typo :: string) :: float;
 local
   aa :: float;
  if typo = "s3" then aa := amplitude(0., 0., "s3"); #``(3·a0)^(-3/2) / sqrt(π);
  elif typo = "p3x" then aa := amplitude((2 - sqrt(2))·a0, 0., "p3x"); #``(3·a0)^(-3/2) / sqrt(3/2·π) · (2 - sqrt(2))
     ·exp(-2 + sqrt(2));
```

```
elif typo = "p3z" then aa := amplitude(0., (2 - sqrt(2))·a0, "p3z"); #``(3·a0)^(-3/2)/sqrt(3/2·π)·(2 - sqrt(2))
·exp(-2 + sqrt(2));
elif typo = "d3z2" then aa := amplitude(0., 6·a0, "d3z2"); #``(3·a0)^(-3/2)/sqrt(6·π)·8·exp(-2);
elif typo = "d3zx" then aa := amplitude(3·sqrt(2)·a0, 3·sqrt(2)·a0, "d3zx"); #``(3·a0)^(-3/2)/sqrt(6·π)·4·exp(
-2);
else aa := 0.00;
end if;
aa := evalf(aa);
return(aa);
end proc: #AmpliMax
```

orbitale "s1"

$$amplitude := \frac{a0^{-\frac{3}{2}}}{\sqrt{\pi}} \cdot \exp\left(-\frac{r}{a0}\right);$$

$$\frac{e^{-\frac{r}{a0}}}{a0^{3/2}\sqrt{\pi}} \tag{1}$$

```
AmpliMax := simplify(subs(r = 0, amplitude))
```

$$\frac{1}{a0^{3/2}\sqrt{\pi}} \tag{2}$$

$$AmpliRel := simplify\left(\frac{amplitude}{AmpliMax}\right)$$

$$e^{-\frac{r}{a0}} \tag{3}$$

$$ProbaRel := subs\left(a0 = 1, r = \sqrt{x^2 + z^2}, simplify\left(AmpliRel^2\right)\right)$$

$$e^{-2\sqrt{x^2 + z^2}} \tag{4}$$

```
plots[contourplot](ProbaRel, x = -4 ..4, z = -4 ..4, filledregions = true, numpoints = 50000, coloring
= ["White", "Maroon"], contours = [0.004, 0.03, 0.15, 0.5]);
```

orbitale "s2"

$$amplitude := \frac{(2\cdot a0)^{-\frac{3}{2}}}{\sqrt{\pi}} \cdot \left(1 - \frac{r}{2\cdot a0}\right) \cdot \exp\left(-\frac{r}{2\cdot a0}\right);$$

$$\frac{1}{4}\,\frac{\sqrt{2}\left(1-\frac{1}{2}\,\frac{r}{a0}\right)e^{-\frac{1}{2}\,\frac{r}{a0}}}{a0^{3/2}\sqrt{\pi}} \tag{5}$$

AmpliMax := simplify(subs(r = 0, amplitude))

$$\frac{1}{4}\,\frac{\sqrt{2}}{a0^{3/2}\sqrt{\pi}} \tag{6}$$

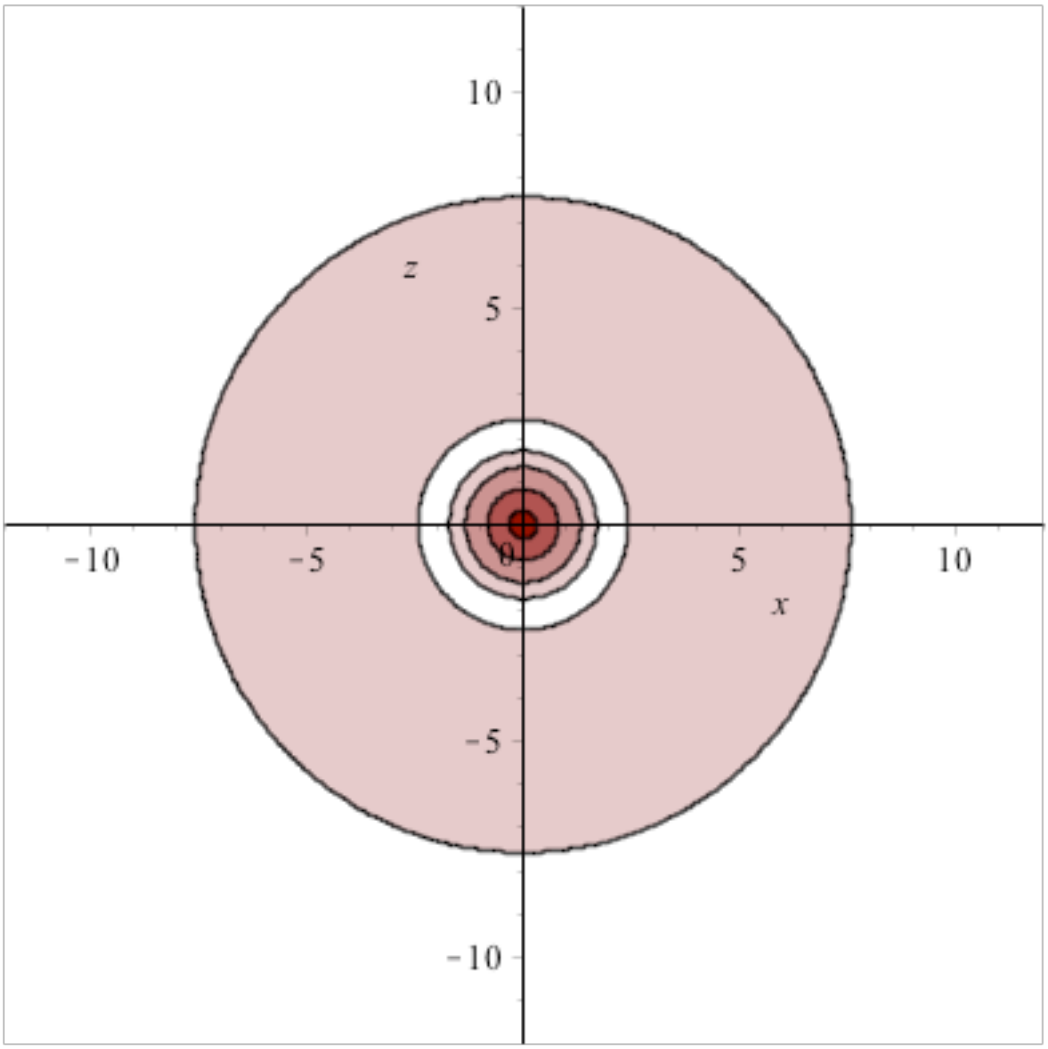
$$AmpliRel := simplify\left(\frac{amplitude}{AmpliMax}\right)$$

$$\frac{1}{2}\,\frac{(2\,a0-r)\,e^{-\frac{1}{2}\,\frac{r}{a0}}}{a0} \tag{7}$$

$$ProbaRel := subs\left(a0 = 1, r = \sqrt{x^2+z^2}, simplify\left(AmpliRel^2\right)\right)$$

$$\frac{1}{4}\left(2-\sqrt{x^2+z^2}\right)^2 e^{-\sqrt{x^2+z^2}} \tag{8}$$

plots[contourplot](*ProbaRel*, x = -12 ..12, z = -12 ..12, filledregions = true, numpoints = 50000, coloring = ["White", "Maroon"], *contours* = [0.004, 0.03, 0.15, 0.5]);



orbitale "p2x"

$$amplitude := \frac{(2\cdot a0)^{-\frac{3}{2}}}{\sqrt{\pi}} \cdot \left(\frac{r}{2\cdot a0}\right) \cdot \exp\left(-\frac{r}{2\cdot a0}\right) \cdot \sin(th);$$

$$\frac{1}{8}\,\frac{\sqrt{2}\,r\,e^{-\frac{1}{2}\,\frac{r}{a0}}\,\sin(th)}{a0^{5/2}\,\sqrt{\pi}} \tag{9}$$

$$\text{AmpliMax} := \text{simplify}\left(\text{subs}\left(\text{r} = 2\cdot\text{a0},\ \text{th} = \frac{\text{Pi}}{2},\ \text{amplitude}\right)\right)$$

$$\frac{1}{4}\,\frac{\sqrt{2}\,e^{-1}}{a0^{3/2}\,\sqrt{\pi}} \tag{10}$$

$$AmpliRel := simplify\left(\frac{amplitude}{AmpliMax}\right)$$

$$\frac{1}{2}\,\frac{r\,\sin(th)\,e^{\frac{1}{2}\,\frac{2\,a0-r}{a0}}}{a0} \tag{11}$$

$$ProbaRel := subs\left(a0 = 1,\ r = \sqrt{x^2+z^2},\ \sin(th) = \frac{|x|}{\sqrt{x^2+z^2}},\ simplify\left(AmpliRel^2\right)\right)$$

$$\frac{1}{4}\,|x|^2\,e^{2-\sqrt{x^2+z^2}} \tag{12}$$

$$plots[contourplot](ProbaRel,\ \text{x} = -12..12,\ \text{z} = -12..12,\ \text{filledregions} = \text{true},\ \text{numpoints} = 50000,$$
$$\text{coloring} = [\text{"White"},\ \text{"Maroon"}],\ contours = [0.004,\ 0.03,\ 0.15,\ 0.5]);$$