

Hydrogen Probability Densities*

for $(n, l, m) = (1, 0, 0)$ **to** $(n, l, m) = (3, 2, 2)$

Point clouds, preferably in stereo, are used to visualize the electron probability densities in a Hydrogen atom. Since these densities are rotationally symmetric around the z -axis, only a wedge of the density cloud is shown.

The Action Menu offers several viewing options:

The entry **Show Coordinate Slices** plays a sequence of coordinate slices, first in polar coordinates, then in Cartesian coordinates.

The entry

Show Constant Density Surface as Point Cloud

shows that surface along which the density has its mean value. One can morph the constant density surfaces with the parameter ff . In some cases these surfaces have several components inside each other. Therefore a stereo point cloud gives a better impression than the raytrace version.

The entry **Show Voxel Raytrace** is the slowest option. It is visually more impressive than the point cloud, but less informative.

The entry **Create** returns to the default volume cloud.

The electron densities are of course listed in Physics texts. For comparison with our visualizations we repeat them here:

* This file is from the 3D-XplorMath project. Please see:

<http://3D-XplorMath.org/>

In 3DXM we use the parameter ii for the Bohr radius a_0 .

$$(n,l,m)=(1,0,0):$$

$$\text{density} := \left(\exp\left(-\frac{r}{a_0}\right) \right)^2,$$

$$(n,l,m)=(2,0,0):$$

$$\text{density} := \left(\left(2 - \frac{r}{a_0}\right) \cdot \exp\left(\frac{-r}{2a_0}\right) \right)^2,$$

$$(n,l,m)=(2,1,0):$$

$$\text{density} := \left(\frac{r}{a_0} \cdot \exp\left(\frac{-r}{2a_0}\right) \cdot \cos \theta \right)^2,$$

$$(n,l,m)=(2,1,1):$$

$$\text{density} := \left(\frac{r}{a_0} \cdot \exp\left(\frac{-r}{2a_0}\right) \cdot \sin \theta \right)^2,$$

$$(n,l,m)=(3,0,0):$$

$$\text{density} := \left(\left(27 - 18\frac{r}{a_0} + 2\left(\frac{r}{a_0}\right)^2\right) \cdot \exp\left(\frac{-r}{3a_0}\right) \right)^2,$$

$$(n,l,m)=(3,1,0):$$

$$\text{density} := \left(\left(6 - \frac{r}{a_0}\right) \cdot \frac{r}{a_0} \cdot \exp\left(\frac{-r}{3a_0}\right) \cdot \cos \theta \right)^2,$$

$$(n,l,m)=(3,1,1):$$

$$\text{density} := \left(\left(6 - \frac{r}{a_0}\right) \cdot \frac{r}{a_0} \cdot \exp\left(\frac{-r}{3a_0}\right) \cdot \sin \theta \right)^2,$$

$$(n,l,m)=(3,2,0):$$

$$\text{density} := \left(\left(\frac{r}{a_0}\right)^2 \cdot \exp\left(\frac{-r}{3a_0}\right) \cdot (3 \cos^2 \theta - 1) \right)^2,$$

$$(n,l,m)=(3,2,1):$$

$$\text{density} := \left(\left(\frac{r}{a_0}\right)^2 \cdot \exp\left(\frac{-r}{3a_0}\right) \cdot \cos \theta \cdot \sin \theta \right)^2,$$

$$(n,l,m)=(3,2,2):$$

$$\text{density} := \left(\left(\frac{r}{a_0}\right)^2 \cdot \exp\left(\frac{-r}{3a_0}\right) \cdot \sin^2 \theta \right)^2,$$

H.K.