

Quantum Mechanics on a Spherical Shell

This is the simplest physical example that uses the “spherical harmonics”.

We imagine that we have a potential of the form

$$V(r) = \lim_{V_0 \rightarrow -\infty} V_0 \delta(R - r)$$

Of course, this is a theorist’s dream, but is closely related to approximations of the potential for the nuclear shell model that we shall encounter in the future.

The Schrödinger equation in 2D spherical coordinates:

$$\begin{aligned}\mathcal{L}^2 Y_{\ell, m_\ell}(\theta, \phi) &= \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y_{\ell, m_\ell}(\theta, \phi) \\ &= \ell(\ell + 1) Y_{\ell, m_\ell}(\theta, \phi)\end{aligned}$$

where

- $\mathcal{L}^2$ is the spherical-polar Laplacian operator
- $Y_{\ell, m_\ell}(\theta, \phi)$ are the spherical harmonics
- ℓ is the orbital quantum number $\ell = 0, 1, 2 \dots$
- m_ℓ is the magnetic quantum number $m_\ell = 0, \pm 1, \pm 2 \dots \pm \ell$
- $\langle Y_{\ell', m'_\ell}(\theta, \phi) Y_{\ell, m_\ell}(\theta, \phi) \rangle = \delta_{\ell', \ell} \delta_{m'_\ell, m_\ell}$ (orthogonality)

Just as $\mathcal{L}^2$ extracts the ℓ quantum number,
the z -component of the ℓ operator, $\mathcal{L}_z$,
extracts the magnetic quantum number m_ℓ , viz.

$$\mathcal{L}_z Y_{\ell, m_\ell}(\theta, \phi) = -i \left(\frac{\partial}{\partial \phi} \right) Y_{\ell, m_\ell}(\theta, \phi) = m_\ell Y_{\ell, m_\ell}(\theta, \phi)$$

Finally, $\hbar^2 \mathcal{L}^2$ is the total angular momentum (squared)
of the particle in orbital ℓ , i.e. $\hbar^2 \ell(\ell + 1)$

and

$\hbar \mathcal{L}_z$ is the z -component of the $\mathcal{L}$ operator in orbital
(ℓ, m_ℓ), i.e. $\hbar m_\ell$

Note that there are no values of ℓ and m_ℓ that result in

$$\langle Y_{\ell, m_\ell}(\theta, \phi) | \mathcal{L}^2 - \mathcal{L}_z^2 | Y_{\ell, m_\ell}(\theta, \phi) \rangle = 0$$

This is a consequence of the Heisenberg Uncertainty relationship for the azimuthal angle

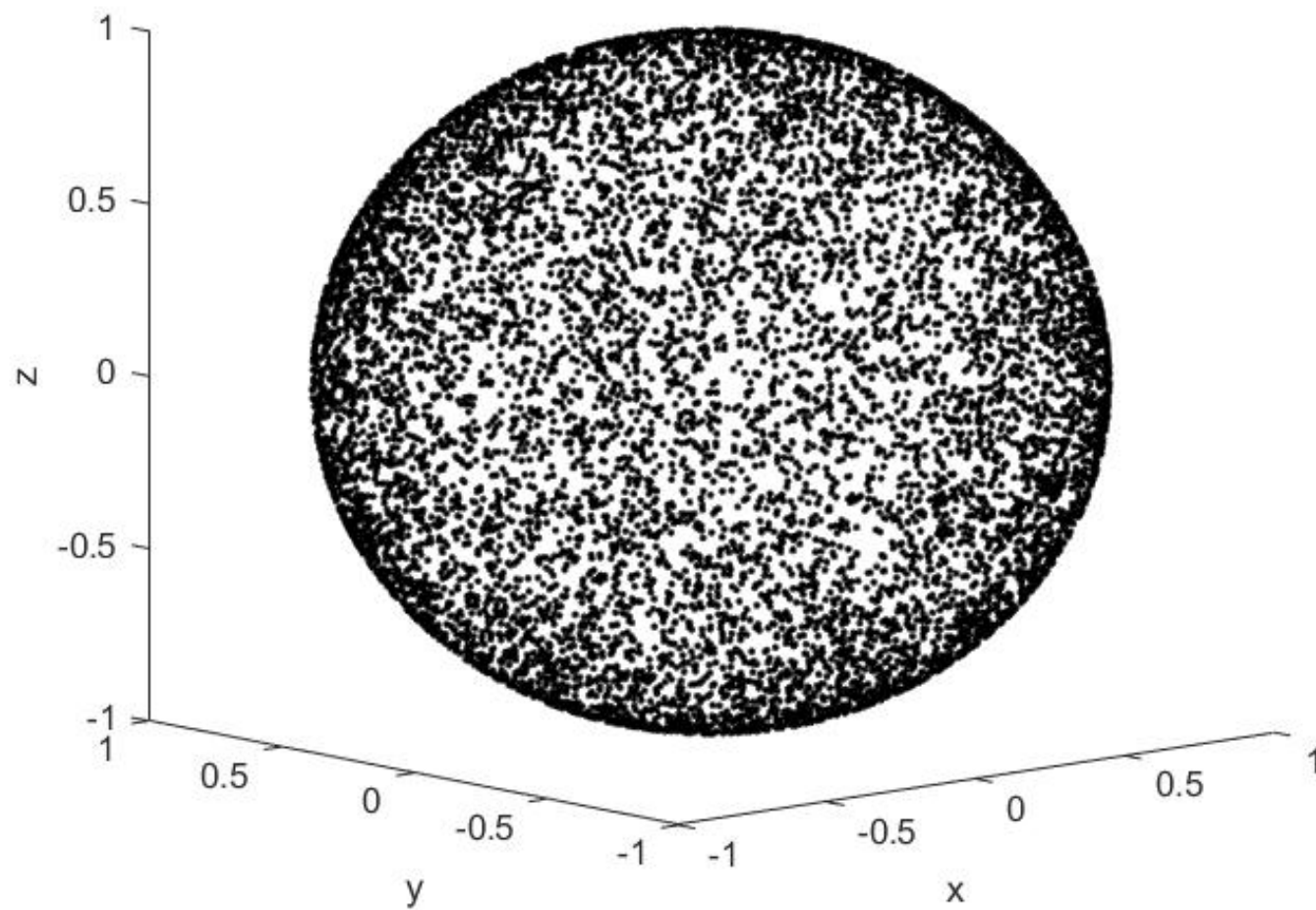
$$\Delta \mathcal{L}_z \Delta \phi \geq \frac{1}{2}$$

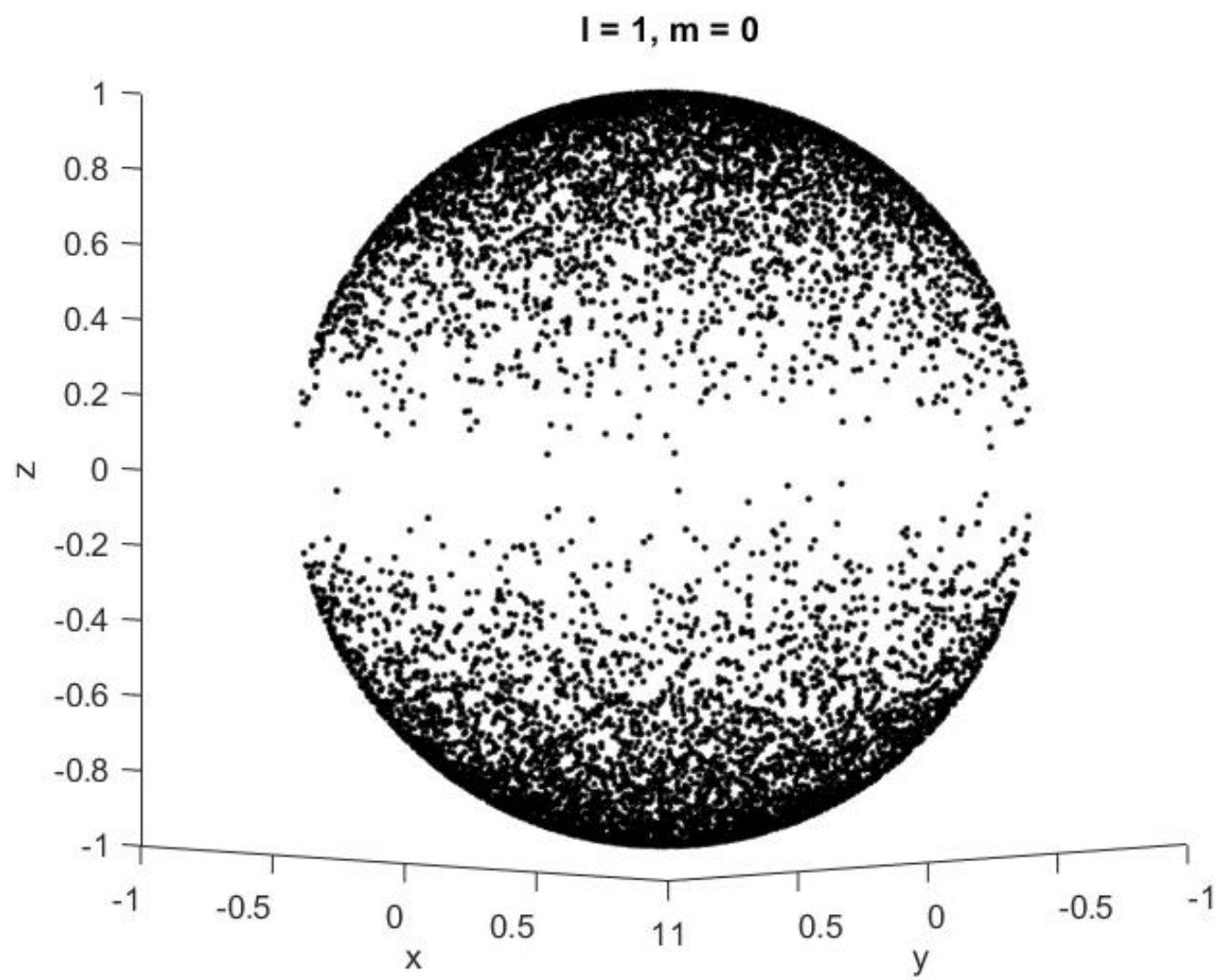
We shall see some effects of these in upcoming plots.

Low-order explicit forms of the $Y_{\ell,m_\ell}(\theta, \phi)$ s:

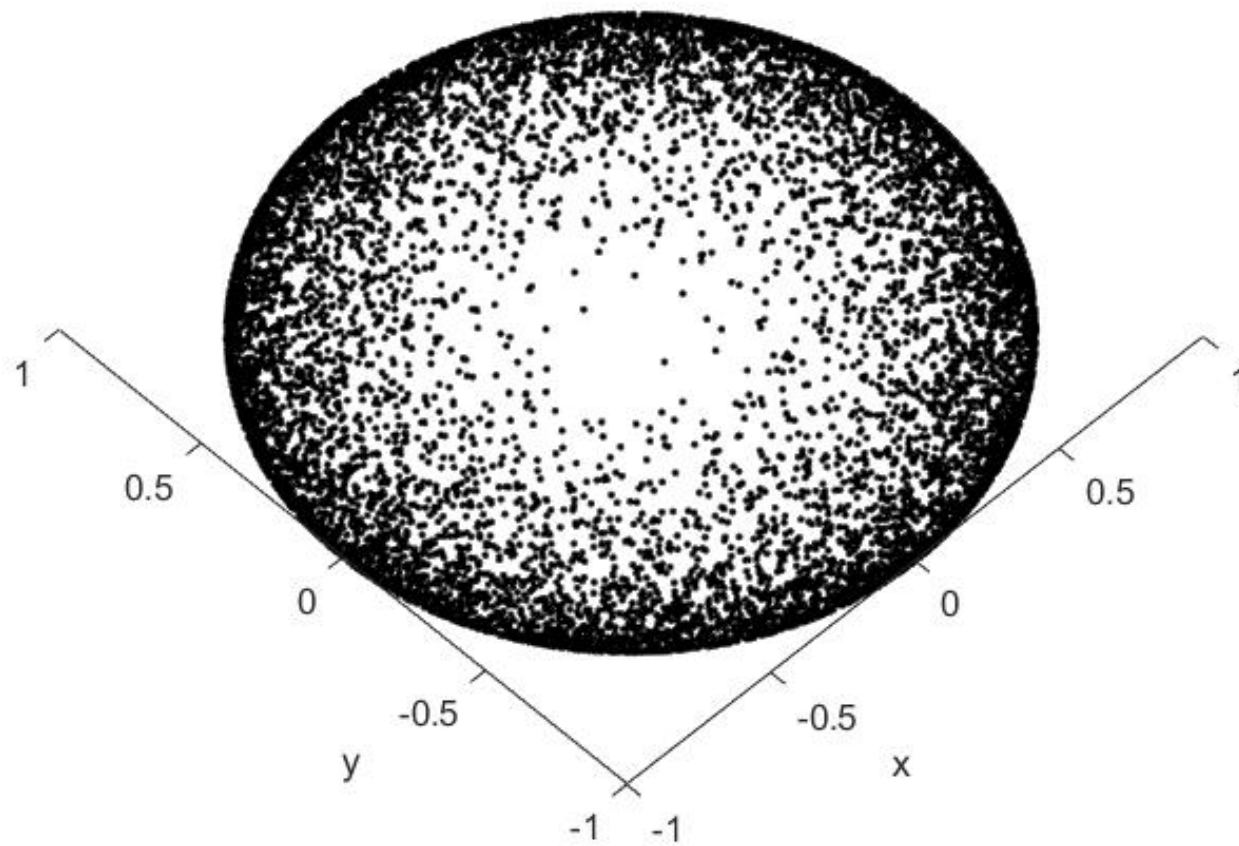
l	m_l	$Y_{\ell,m_\ell}(\theta, \phi)$
0	0	$(\frac{1}{4\pi})^{1/2}$
1	0	$(\frac{3}{4\pi})^{1/2} \cos \theta$
1	± 1	$\mp (\frac{3}{8\pi})^{1/2} \sin \theta e^{\pm i\phi}$
2	0	$(\frac{5}{16\pi})^{1/2} (3 \cos^2 \theta - 1)$
2	± 1	$\mp (\frac{15}{8\pi})^{1/2} \sin \theta \cos \theta e^{\pm i\phi}$
2	± 2	$(\frac{15}{32\pi})^{1/2} \sin^2 \theta e^{\pm i2\phi}$
$\vdots$	$\vdots$	$\vdots$

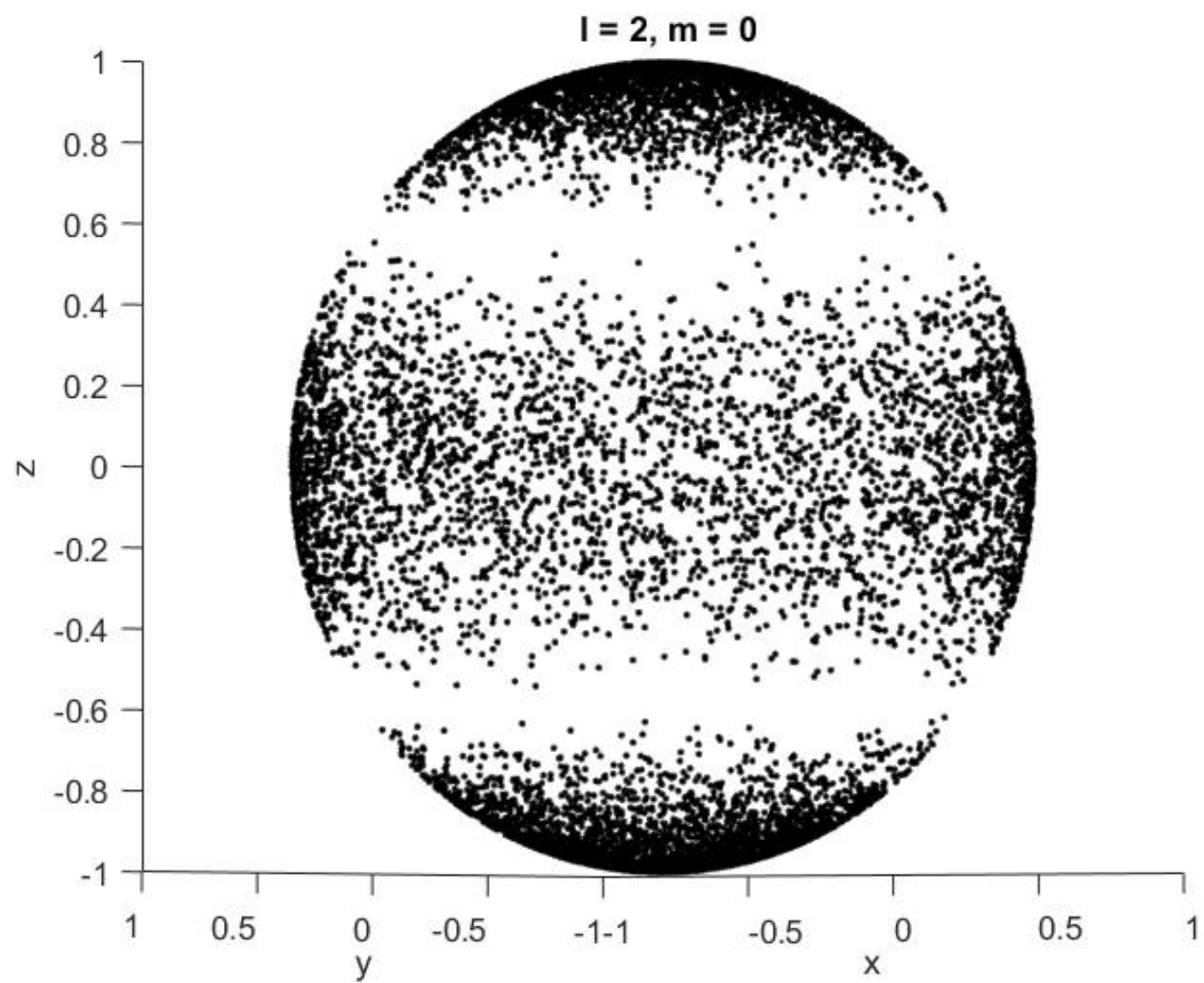
$l = 0, m = 0$

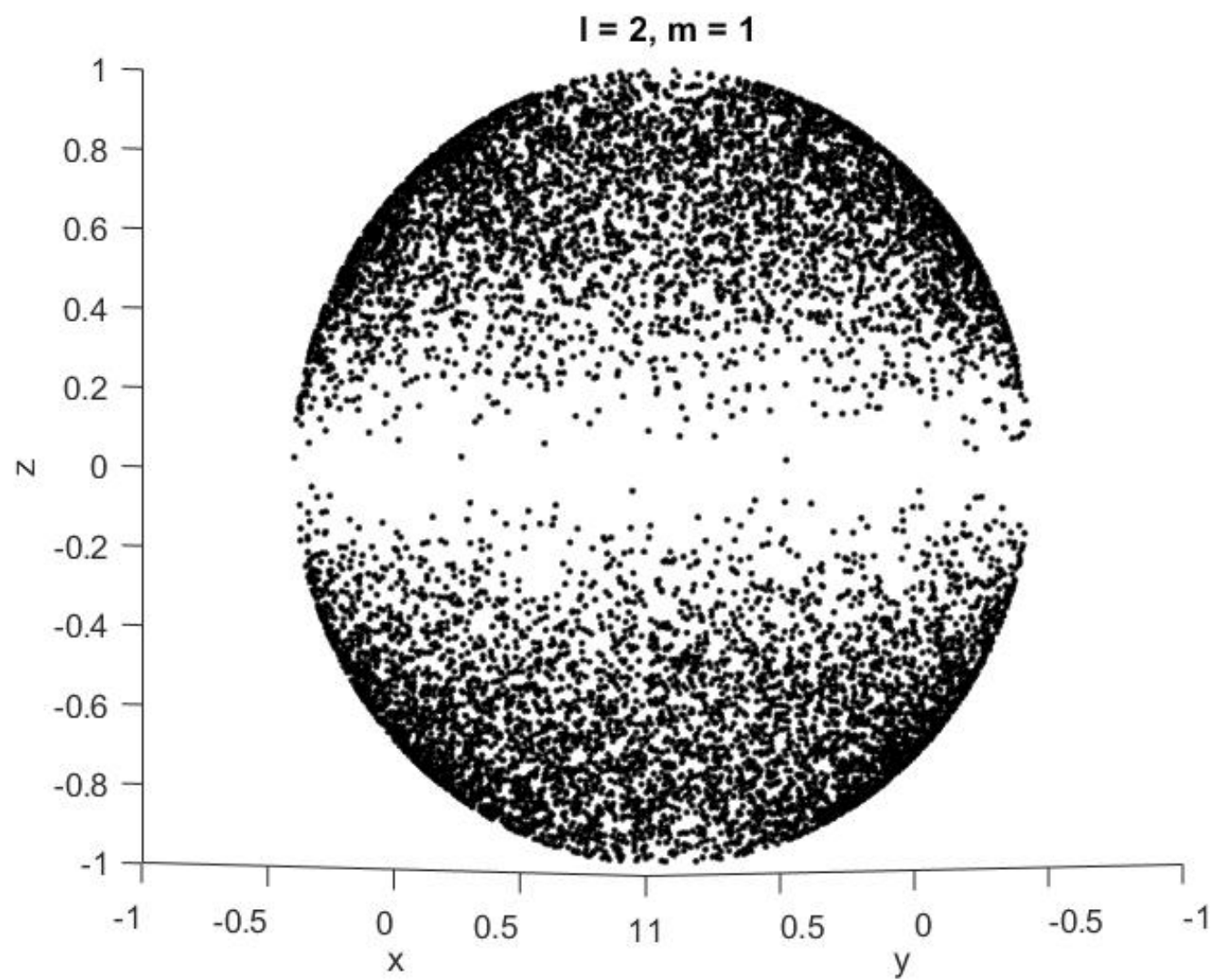




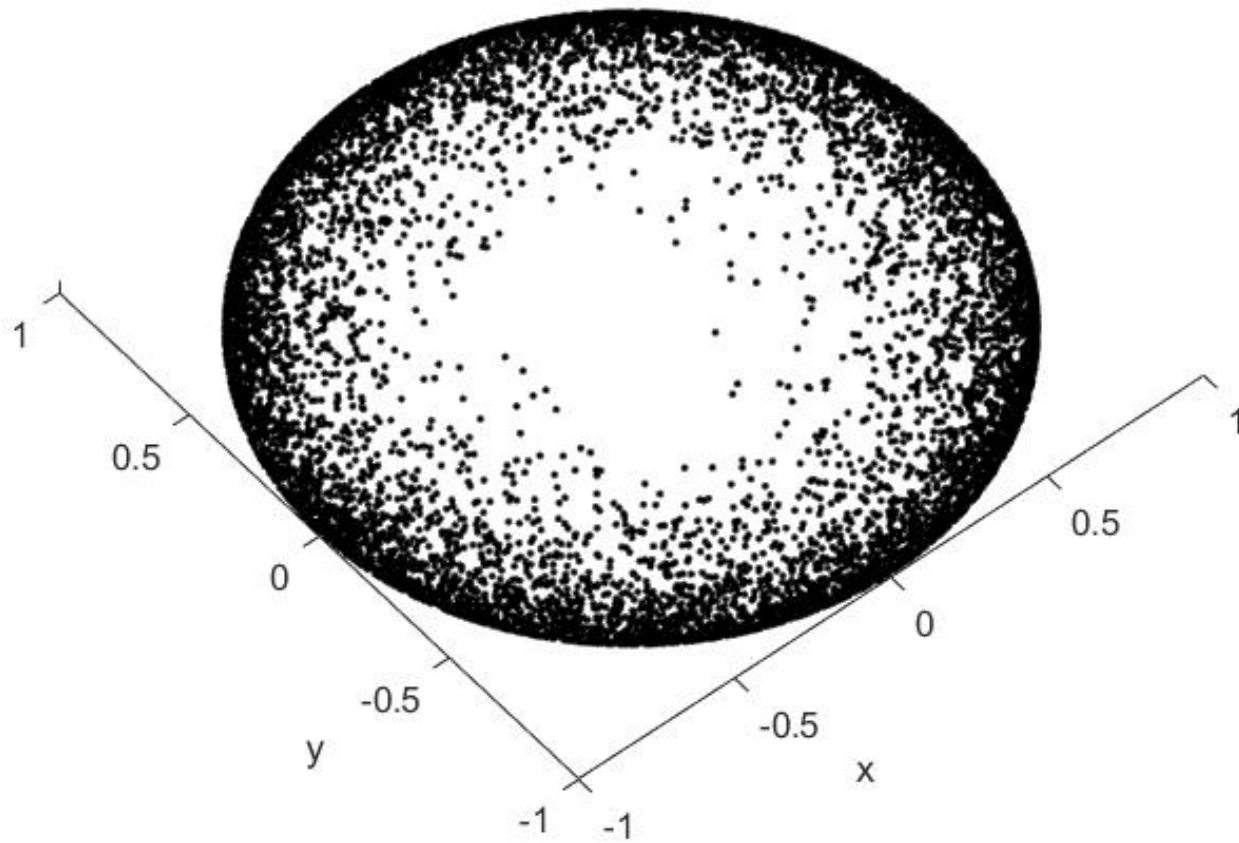
$l = 1, m = 1$







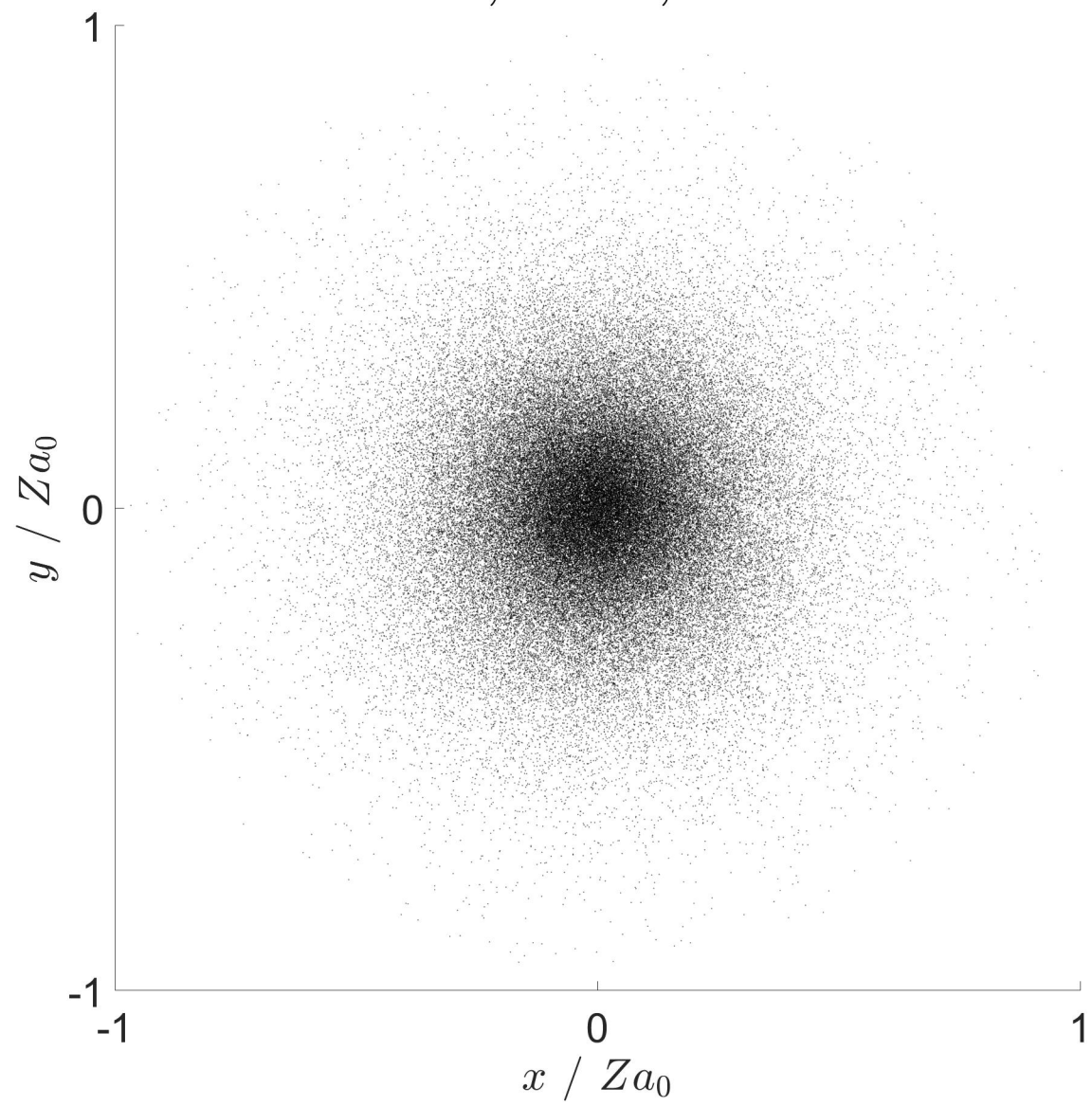
$l = 2, m = 2$



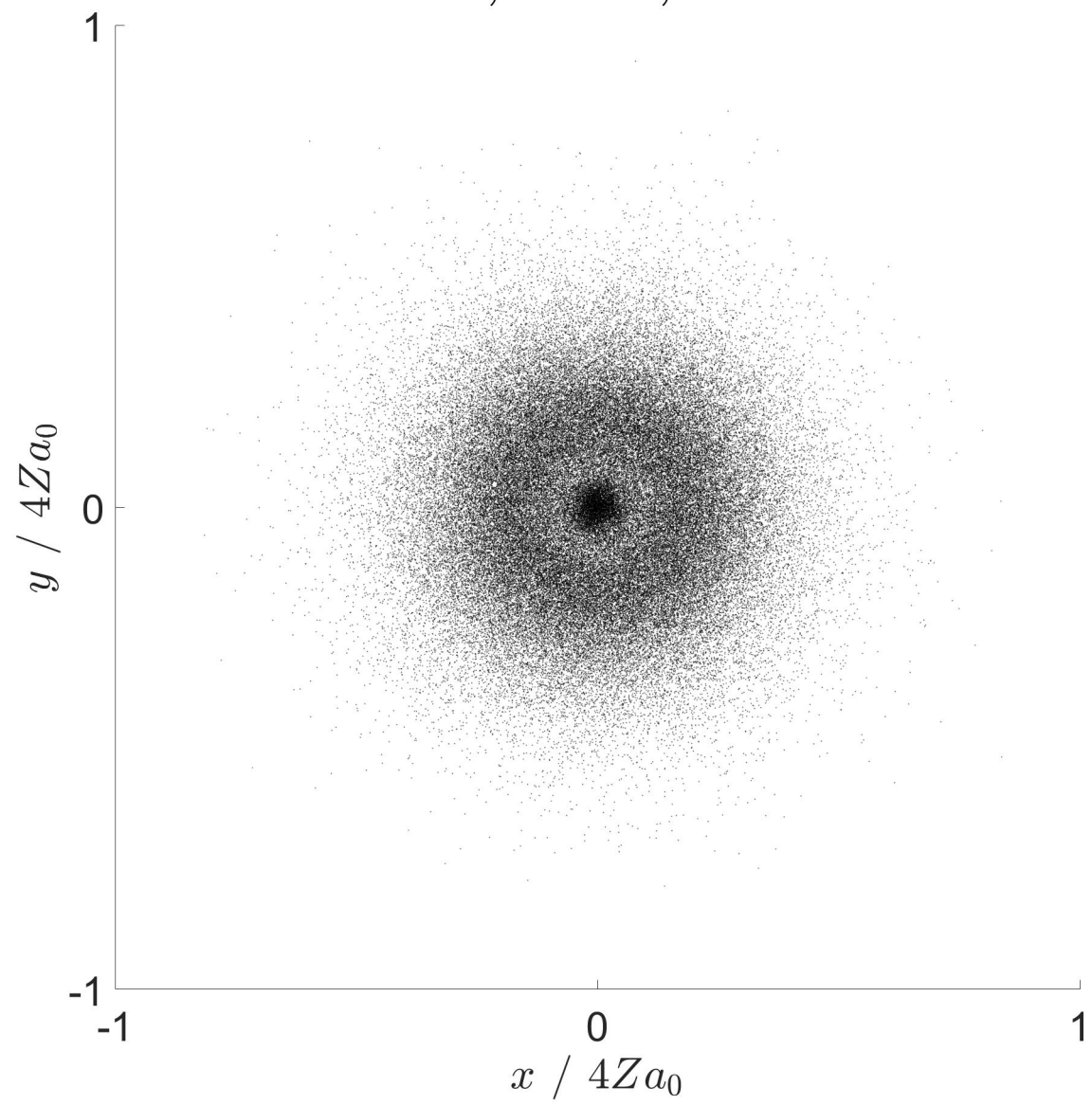
Spherical Harmonics and Hydrogenic wavefunctions

On the next few slides you can see the effect of the spherical harmonics on the hydrogenic wavefunctions(Z protons in the nucleus, with only one e^- in “orbit”).

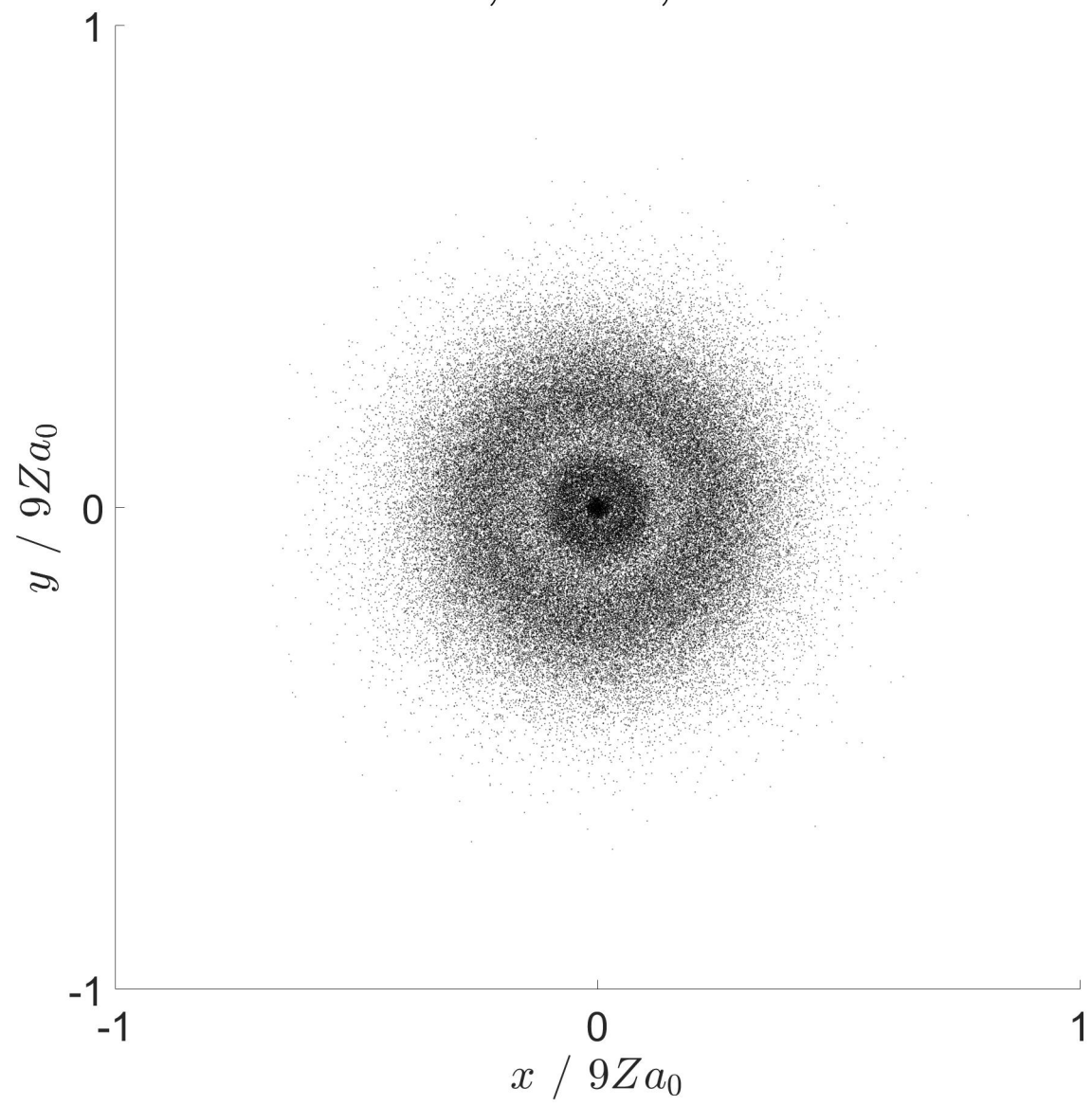
$$n = 1, l = 0, m = 0$$



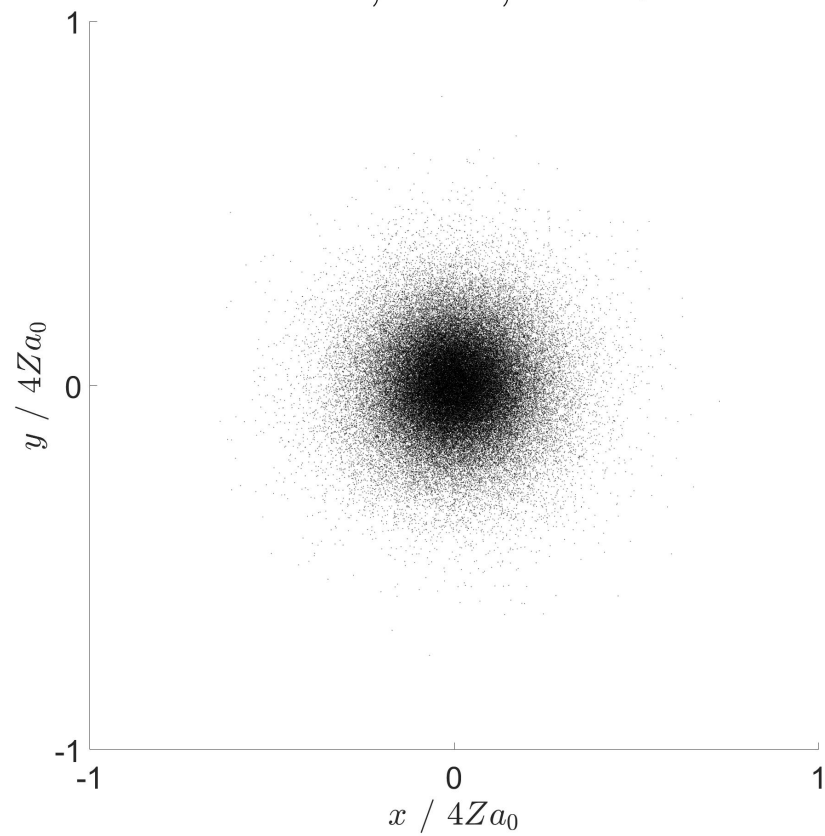
$$n = 2, l = 0, m = 0$$



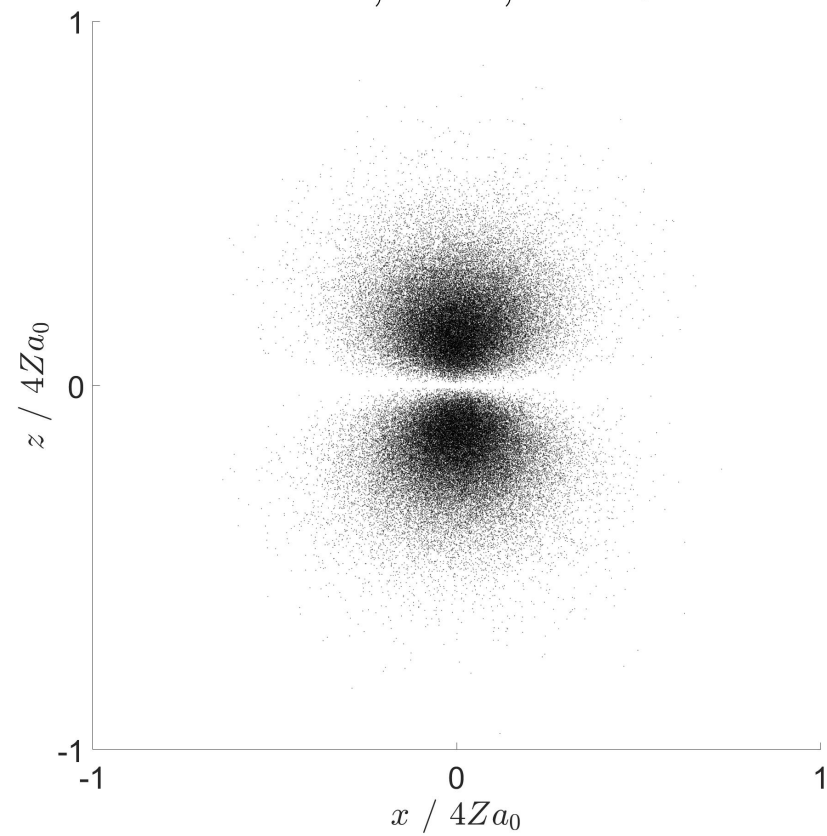
$$n = 3, l = 0, m = 0$$



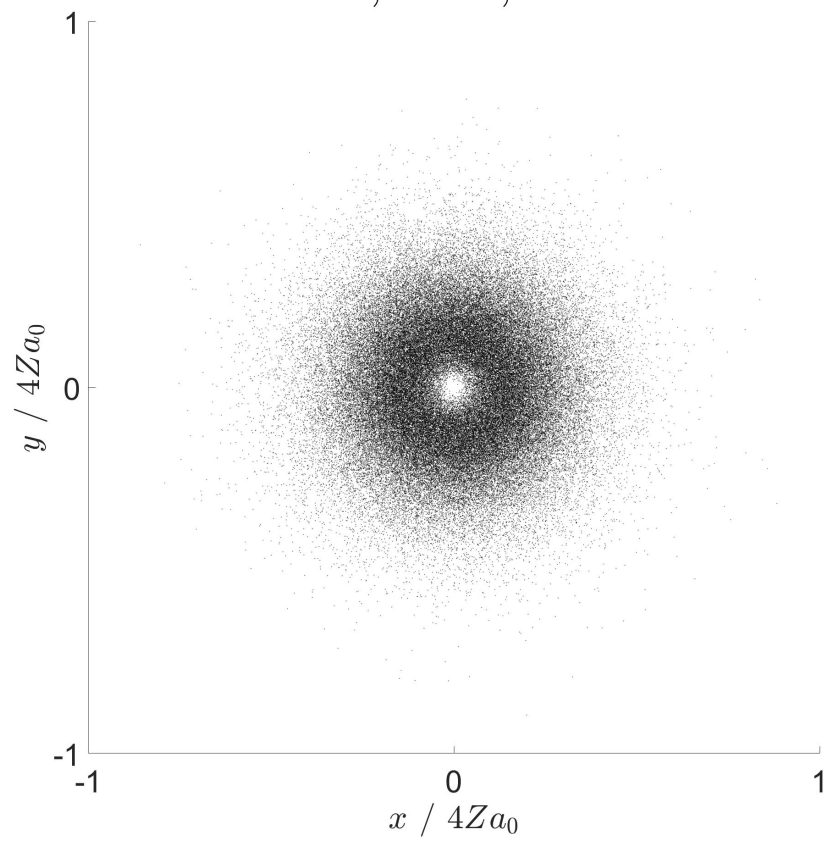
$n = 2, l = 1, m = 0$



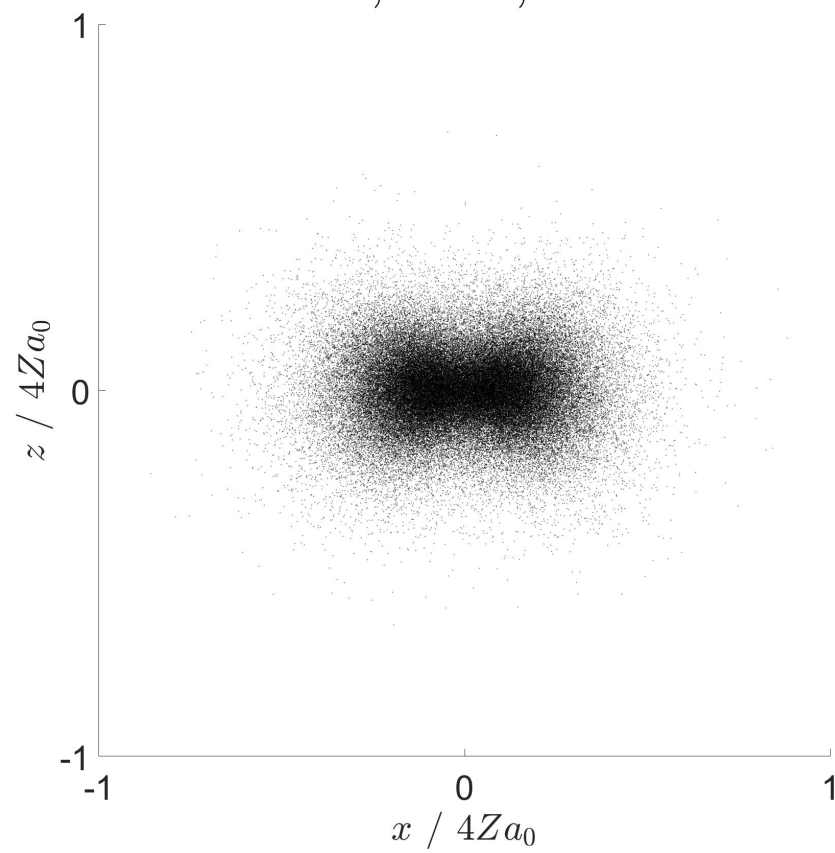
$n = 2, l = 1, m = 0$



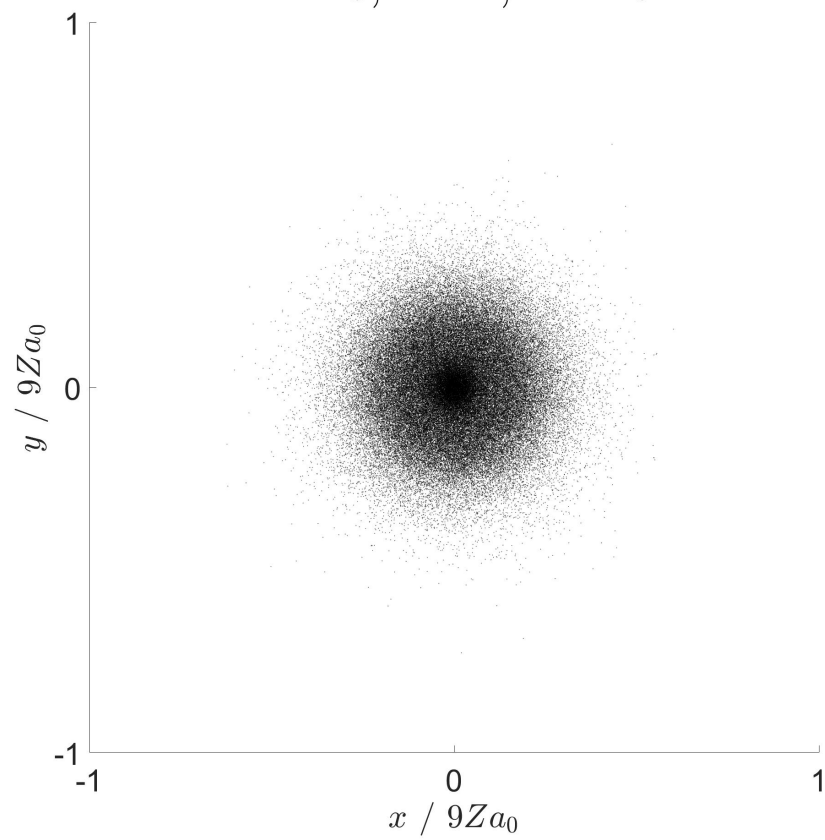
$n = 2, l = 1, m = 1$



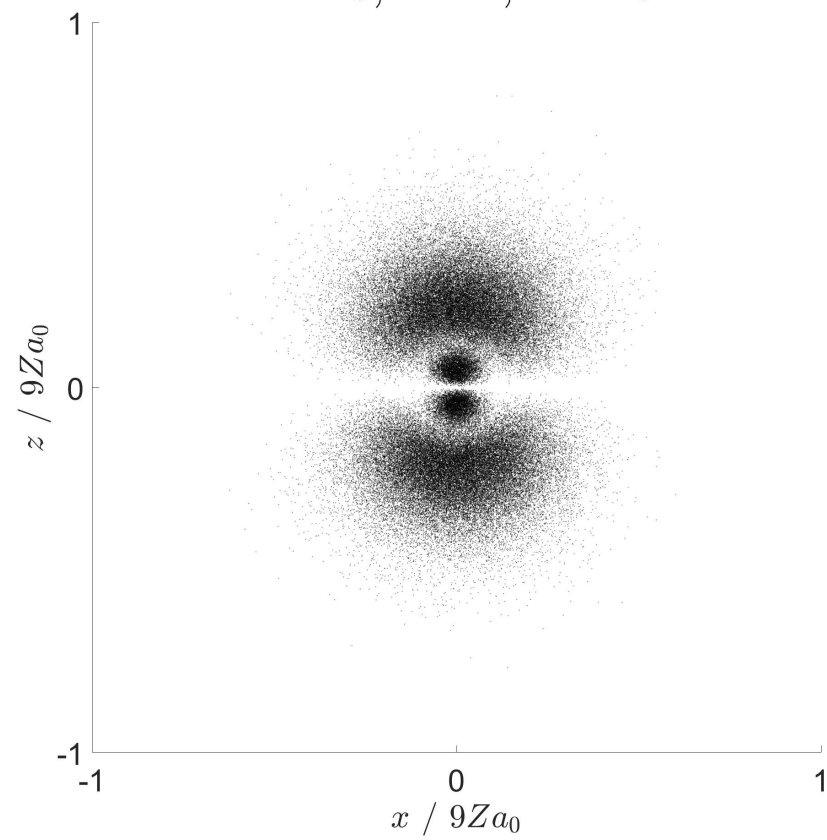
$n = 2, l = 1, m = 1$



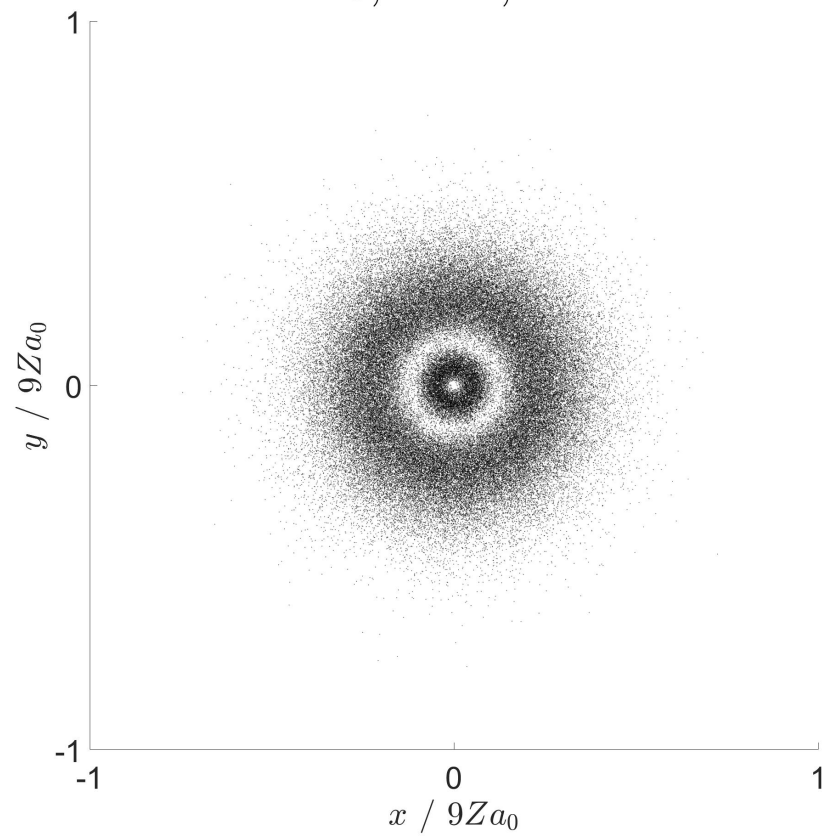
$n = 3, l = 1, m = 0$



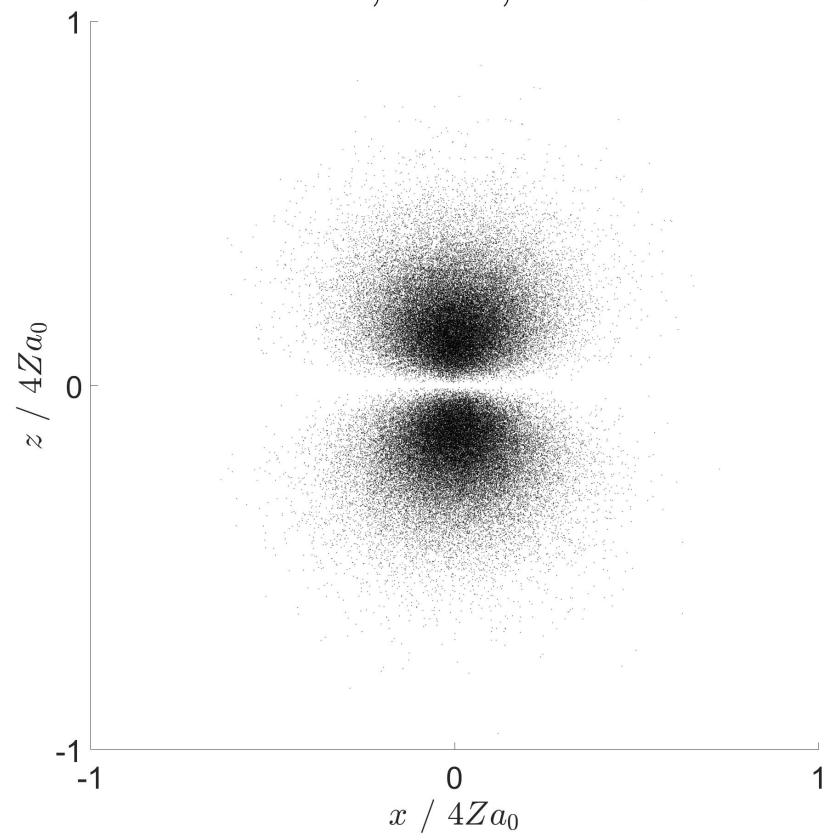
$n = 3, l = 1, m = 0$



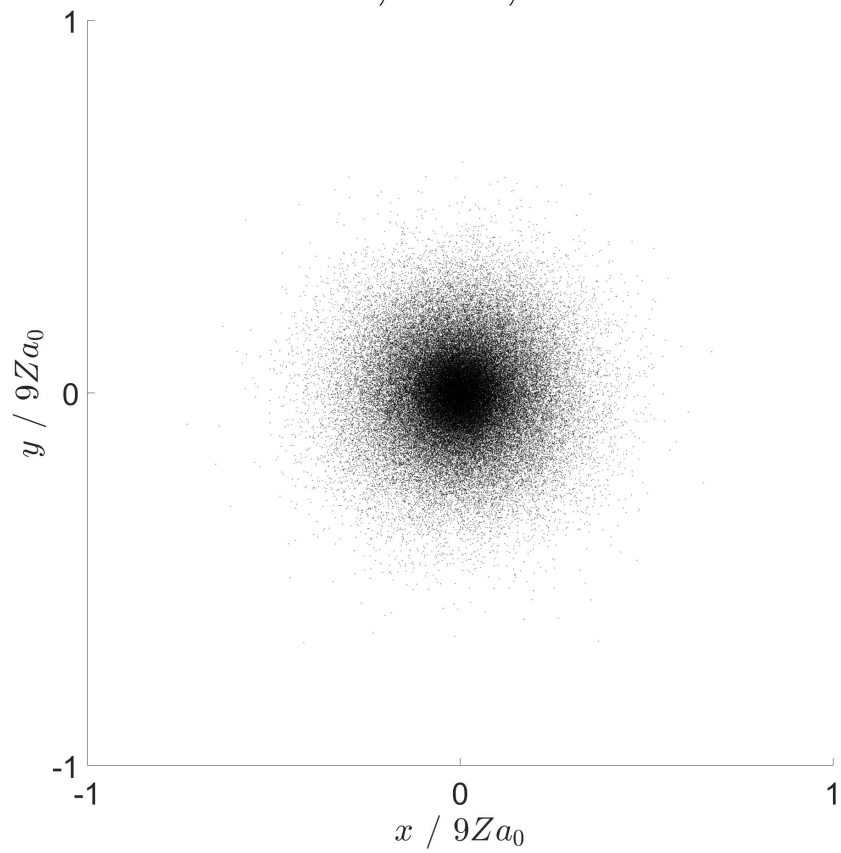
$n = 3, l = 1, m = 1$



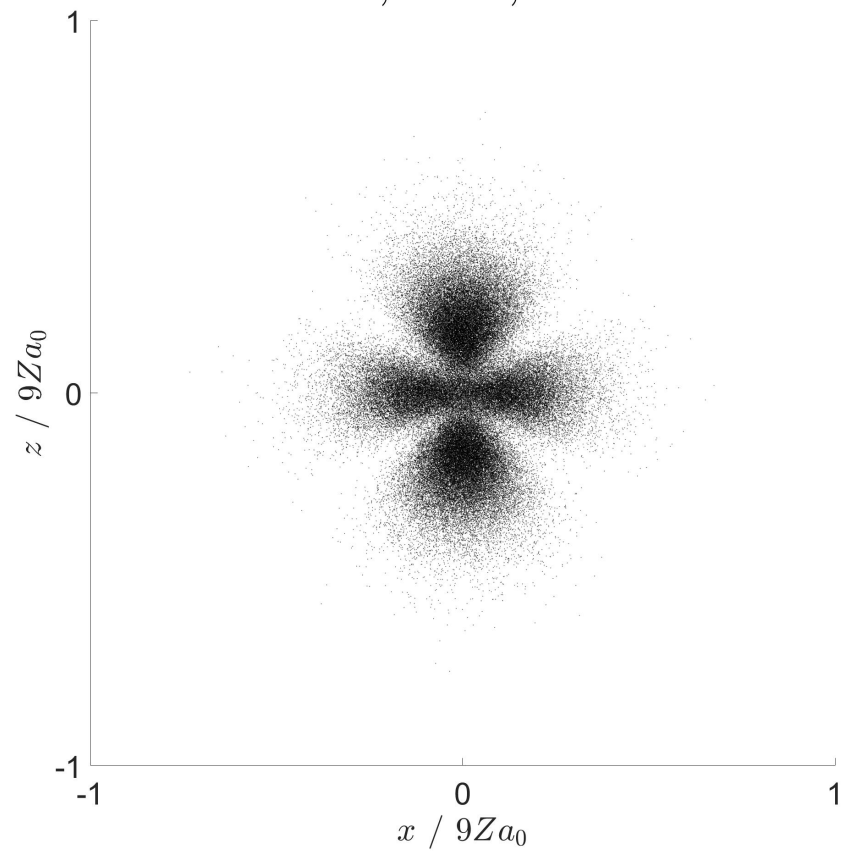
$n = 2, l = 1, m = 0$



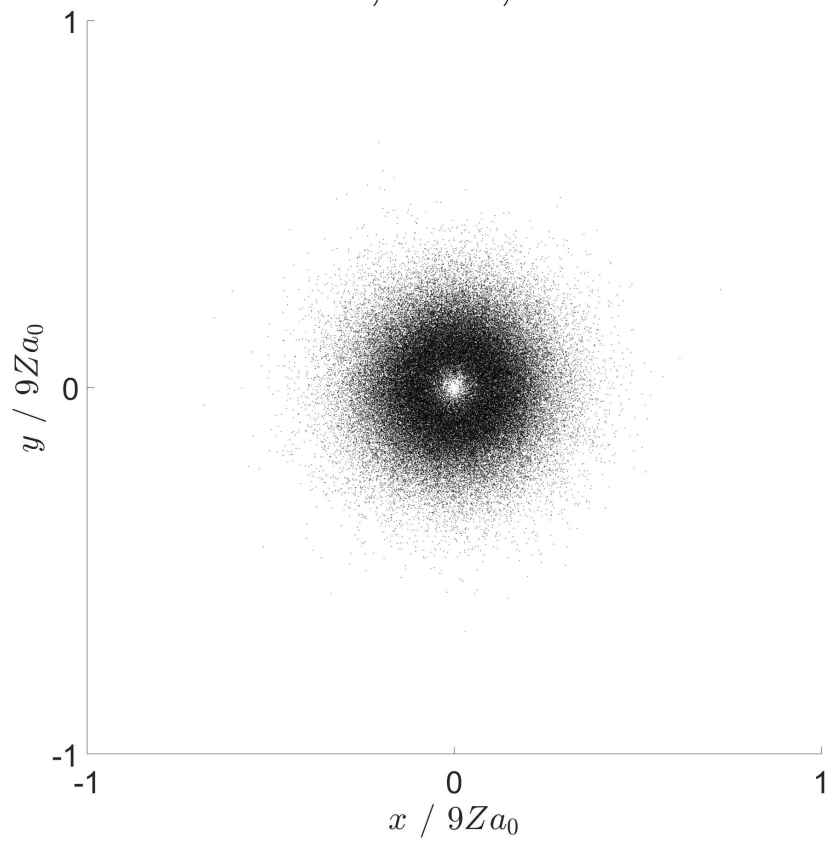
$n = 3, l = 2, m = 0$



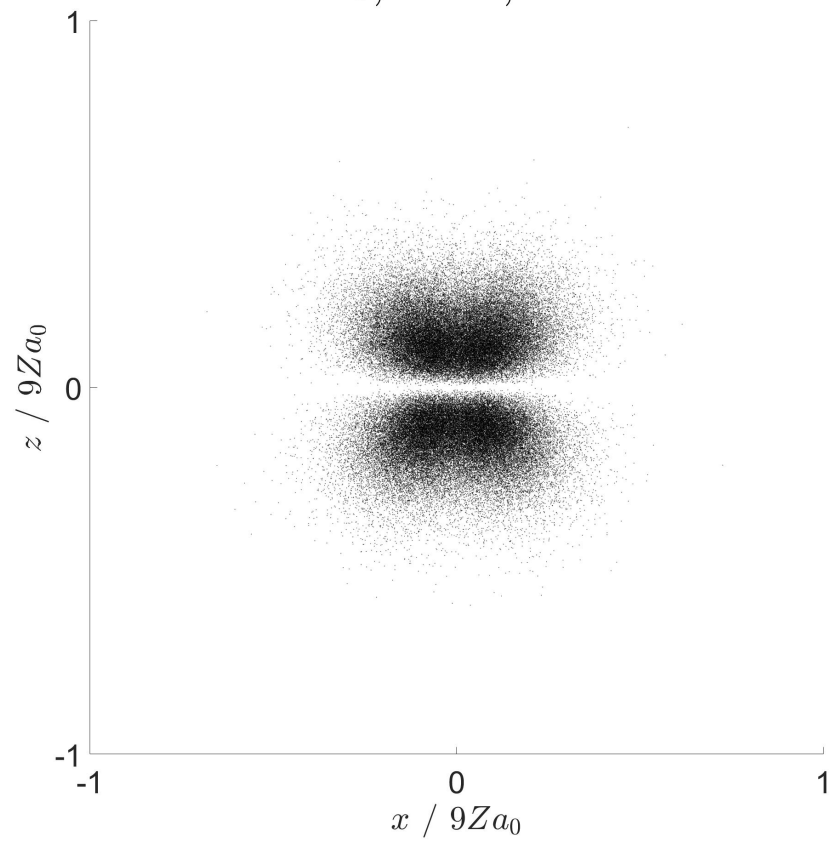
$n = 3, l = 2, m = 0$



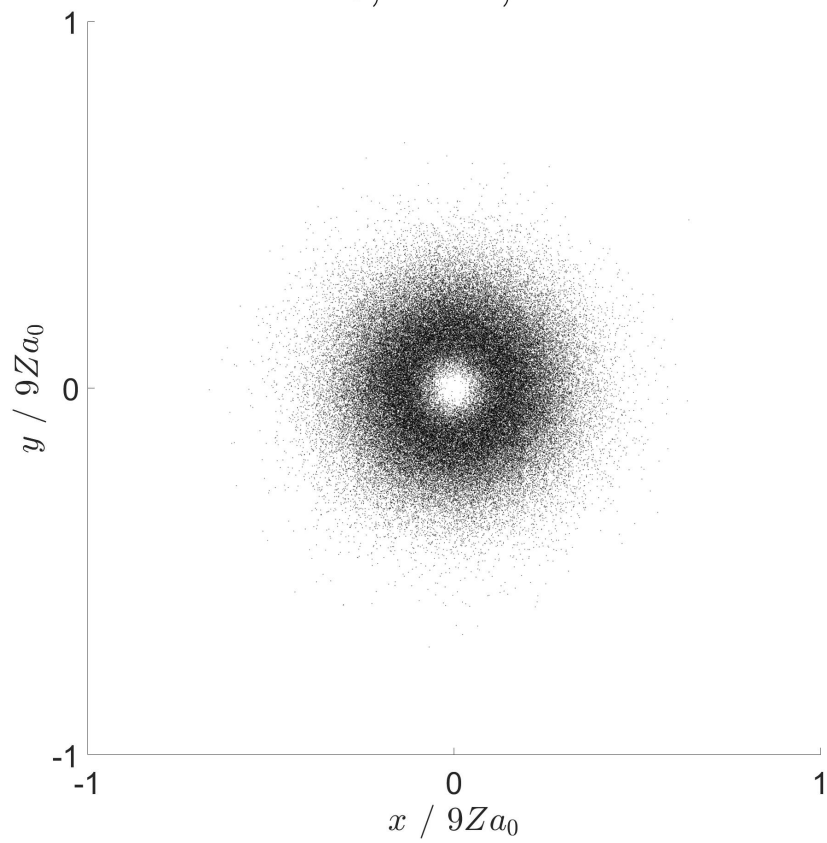
$n = 3, l = 2, m = 1$



$n = 3, l = 2, m = 1$



$n = 3, l = 2, m = 2$



$n = 3, l = 2, m = 2$

