

## SymPy generated orbital functions

Orbitals are constructed in the following fashion:

$$\phi(\vec{r})_{n,l,m} = L_{n-l-1}^{2l+1} \left( \frac{2r}{n} k \right) S_l^m(\vec{r}) e^{-\frac{r}{n}k}$$

where  $n$  is the principal quantum number,  $k = \alpha Z$  with  $Z$  being the nucleus charge and  $\alpha$  being the variational parameter.

$$l = 0, 1, \dots, (n-1)$$

$$m = -l, (-l+1), \dots, (l-1), l$$

$\phi_0 \rightarrow \phi_{1,0,0}$	
$\phi(\vec{r})$	1
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kx}{r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{ky}{r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz}{r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(kr-2)}{r}$

Table 1: Orbital expressions hydrogenicOrbitals : 1, 0, 0. Factor  $e^{-kr}$  is omitted.

$\phi_1 \rightarrow \phi_{2,0,0}$	
$\phi(\vec{r})$	$kr - 2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kx(kr-4)}{2r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{ky(kr-4)}{2r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz(kr-4)}{2r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(kr-8)(kr-2)}{4r}$

Table 2: Orbital expressions hydrogenicOrbitals : 2, 0, 0. Factor  $e^{-\frac{1}{2}kr}$  is omitted.

$\phi_2 \rightarrow \phi_{2,1,0}$	
$\phi(\vec{r})$	$z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz}{2r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kyz}{2r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz^2+2r}{2r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kz(kr-8)}{4r}$

Table 3: Orbital expressions hydrogenicOrbitals : 2, 1, 0. Factor  $e^{-\frac{1}{2}kr}$  is omitted.

$\phi_3 \rightarrow \phi_{2,1,1}$	
$\phi(\vec{r})$	$x$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kx^2+2r}{2r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy}{2r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz}{2r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kx(kr-8)}{4r}$

Table 4: Orbital expressions hydrogenicOrbitals : 2, 1, 1. Factor  $e^{-\frac{1}{2}kr}$  is omitted.

$\phi_4 \rightarrow \phi_{2,1,-1}$	
$\phi(\vec{r})$	$y$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy}{2r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{ky^2+2r}{2r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kyz}{2r}$
$\nabla^2 \phi(\vec{r})$	$\frac{ky(kr-8)}{4r}$

Table 5: Orbital expressions hydrogenicOrbitals : 2, 1, -1. Factor  $e^{-\frac{1}{2}kr}$  is omitted.

$\phi_5 \rightarrow \phi_{3,0,0}$	
$\phi(\vec{r})$	$2k^2r^2 - 18kr + 27$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kx(2k^2r^2-30kr+81)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{ky(2k^2r^2-30kr+81)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz(2k^2r^2-30kr+81)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(kr-18)(2k^2r^2-18kr+27)}{9r}$

Table 6: Orbital expressions hydrogenicOrbitals : 3, 0, 0. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_6 \rightarrow \phi_{3,1,0}$	
$\phi(\vec{r})$	$z (kr - 6)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz(kr-9)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kzy(kr-9)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$\frac{3kr^2 - kz^2(kr-9) - 18r}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kz(kr-18)(kr-6)}{9r}$

Table 7: Orbital expressions hydrogenicOrbitals : 3, 1, 0. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_7 \rightarrow \phi_{3,1,1}$	
$\phi(\vec{r})$	$x (kr - 6)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$\frac{3kr^2 - kx^2(kr-9) - 18r}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy(kr-9)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz(kr-9)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kx(kr-18)(kr-6)}{9r}$

Table 8: Orbital expressions hydrogenicOrbitals : 3, 1, 1. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_8 \rightarrow \phi_{3,1,-1}$	
$\phi(\vec{r})$	$y (kr - 6)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy(kr-9)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$\frac{3kr^2 - ky^2(kr-9) - 18r}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kzy(kr-9)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{ky(kr-18)(kr-6)}{9r}$

Table 9: Orbital expressions hydrogenicOrbitals : 3, 1, -1. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_9 \rightarrow \phi_{3,2,0}$	
$\phi(\vec{r})$	$-r^2 + 3z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{x(k(-r^2+3z^2)+6r)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{y(k(-r^2+3z^2)+6r)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{z(k(-r^2+3z^2)-12r)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(-r^2+3z^2)(kr-18)}{9r}$

Table 10: Orbital expressions hydrogenicOrbitals : 3, 2, 0. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_{10} \rightarrow \phi_{3,2,1}$	
$\phi(\vec{r})$	$xz$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{z(kx^2-3r)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kxyz}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{x(kz^2-3r)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kxz(kr-18)}{9r}$

Table 11: Orbital expressions hydrogenicOrbitals : 3, 2, 1. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_{11} \rightarrow \phi_{3,2,-1}$	
$\phi(\vec{r})$	$yz$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxyz}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{z(ky^2-3r)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{y(kz^2-3r)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kxyz(kr-18)}{9r}$

Table 12: Orbital expressions hydrogenicOrbitals : 3, 2, -1. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_{12} \rightarrow \phi_{3,2,2}$	
$\phi(\vec{r})$	$x^2 - y^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{x(k(x^2 - y^2) - 6r)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{y(k(x^2 - y^2) + 6r)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz(x^2 - y^2)}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(x^2 - y^2)(kr - 18)}{9r}$

Table 13: Orbital expressions hydrogenicOrbitals : 3, 2, 2. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_{13} \rightarrow \phi_{3,2,-2}$	
$\phi(\vec{r})$	$xy$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{y(kx^2 - 3r)}{3r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{x(ky^2 - 3r)}{3r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kxyz}{3r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kxy(kr - 18)}{9r}$

Table 14: Orbital expressions hydrogenicOrbitals : 3, 2, -2. Factor  $e^{-\frac{1}{3}kr}$  is omitted.

$\phi_{14} \rightarrow \phi_{4,0,0}$	
$\phi(\vec{r})$	$k^3 r^3 - 24k^2 r^2 + 144kr - 192$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kx(k^3 r^3 - 36k^2 r^2 + 336kr - 768)}{4r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{ky(k^3 r^3 - 36k^2 r^2 + 336kr - 768)}{4r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kz(k^3 r^3 - 36k^2 r^2 + 336kr - 768)}{4r}$
$\nabla^2 \phi(\vec{r})$	$\frac{k(kr - 32)(k^3 r^3 - 24k^2 r^2 + 144kr - 192)}{16r}$

Table 15: Orbital expressions hydrogenicOrbitals : 4, 0, 0. Factor  $e^{-\frac{1}{4}kr}$  is omitted.

$\phi_{15} \rightarrow \phi_{4,1,0}$	
$\phi(\vec{r})$	$z(k^2 r^2 - 20kr + 80)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz(kr-20)(kr-8)}{4r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kyz(kr-20)(kr-8)}{4r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$\frac{4k^2 r^3 - 80kr^2 - kz^2(kr-20)(kr-8) + 320r}{4r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kz(kr-32)(k^2 r^2 - 20kr + 80)}{16r}$

Table 16: Orbital expressions hydrogenicOrbitals : 4, 1, 0. Factor  $e^{-\frac{1}{4}kr}$  is omitted.

$\phi_{16} \rightarrow \phi_{4,1,1}$	
$\phi(\vec{r})$	$x(k^2 r^2 - 20kr + 80)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$\frac{4k^2 r^3 - 80kr^2 - kx^2(kr-20)(kr-8) + 320r}{4r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy(kr-20)(kr-8)}{4r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kxz(kr-20)(kr-8)}{4r}$
$\nabla^2 \phi(\vec{r})$	$\frac{kx(kr-32)(k^2 r^2 - 20kr + 80)}{16r}$

Table 17: Orbital expressions hydrogenicOrbitals : 4, 1, 1. Factor  $e^{-\frac{1}{4}kr}$  is omitted.

$\phi_{17} \rightarrow \phi_{4,1,-1}$	
$\phi(\vec{r})$	$y(k^2 r^2 - 20kr + 80)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-\frac{kxy(kr-20)(kr-8)}{4r}$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$\frac{4k^2 r^3 - 80kr^2 - ky^2(kr-20)(kr-8) + 320r}{4r}$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-\frac{kyz(kr-20)(kr-8)}{4r}$
$\nabla^2 \phi(\vec{r})$	$\frac{ky(kr-32)(k^2 r^2 - 20kr + 80)}{16r}$

Table 18: Orbital expressions hydrogenicOrbitals : 4, 1, -1. Factor  $e^{-\frac{1}{4}kr}$  is omitted.