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 α being the variational parameter.

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

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

$\phi_0 \to \phi_{1,0,0}$	
$\phi(\vec{r})$	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.

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

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

$\phi_2 \to \phi_{2,1,0}$	
$\phi(\vec{r})$	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.

$\phi_3 \to \phi_{2,1,1}$	
$\phi(\vec{r})$	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.

$\phi_4 \to \phi_{2,1,-1}$	
$\phi(\vec{r})$	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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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