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
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-\frac{kx}{r}$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-\frac{ky}{r}$
$\vec{k} \cdot \nabla\phi(\vec{r})$	$-\frac{kz}{r}$
$\nabla^2\phi(\vec{r})$	$\frac{k}{r}\left(kr-2\right)$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\phi_{16} \to \phi_{4,1,1}$	
$\phi(\vec{r})$	$-x\left(k^2r^2 - 20kr + 80\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$\frac{1}{4r}\left(k^3r^2x^2 - 4k^2r\left(r^2 + 7x^2\right) + 80k\left(r^2 + 2x^2\right) - 320r\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$\frac{kxy}{4r}\left(kr - 20\right)\left(kr - 8\right)$
$\vec{k} \cdot \nabla\phi(\vec{r})$	$\frac{kxz}{4r}\left(kr - 20\right)\left(kr - 8\right)$
$\nabla^2\phi(\vec{r})$	$-\frac{kx}{16r}\left(kr - 32\right)\left(k^2r^2 - 20kr + 80\right)$

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

$\phi_{17} \to \phi_{4,1,-1}$	
$\phi(\vec{r})$	$-y\left(k^2r^2 - 20kr + 80\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$\frac{kxy}{4r}\left(kr - 20\right)\left(kr - 8\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$\frac{1}{4r}\left(k^3r^2y^2 - 4k^2r\left(r^2 + 7y^2\right) + 80k\left(r^2 + 2y^2\right) - 320r\right)$
$\vec{k} \cdot \nabla\phi(\vec{r})$	$\frac{kyz}{4r}\left(kr - 20\right)\left(kr - 8\right)$
$\nabla^2\phi(\vec{r})$	$-\frac{ky}{16r}\left(kr - 32\right)\left(k^2r^2 - 20kr + 80\right)$

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