# 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.

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

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

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

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.

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

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.

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

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

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

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

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

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

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

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