SymPy generated orbital functions

Orbitals are constructed in the following fashion:

$$\phi(\vec{r})_{n_x,n_y} = H_{n_x}(kx)H_{n_y}(ky)e^{-\frac{1}{2}k^2r^2}$$

where $k = \omega\alpha$, with ω being the oscillator frequency and α being the variational parameter.

$H_0(kx)$	1
$H_1(kx)$	$2kx$
$H_2(kx)$	$4k^2x^2 - 2$
$H_3(kx)$	$8k^3x^3 - 12kx$
$H_4(kx)$	$16k^4x^4 - 48k^2x^2 + 12$
$H_5(kx)$	$32k^5x^5 - 160k^3x^3 + 120kx$
$H_0(ky)$	1
$H_1(ky)$	$2ky$
$H_2(ky)$	$4k^2y^2 - 2$
$H_3(ky)$	$8k^3y^3 - 12ky$
$H_4(ky)$	$16k^4y^4 - 48k^2y^2 + 12$
$H_5(ky)$	$32k^5y^5 - 160k^3y^3 + 120ky$

Table 1: Hermite polynomials used to construct orbital functions

$\phi_0 \to \phi_{0,0}$	
$\phi(\vec{r})$	1
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2 x$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2 y$
$\nabla^2\phi(\vec{r})$	$k^2 \left(k^2 r^2 - 2\right)$

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

$\phi_1 \to \phi_{0,1}$	
$\phi(\vec{r})$	y
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2 xy$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-\left(ky - 1\right)\left(ky + 1\right)$
$\nabla^2\phi(\vec{r})$	$k^2 y \left(k^2 r^2 - 4\right)$

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

$\phi_2 \to \phi_{1,0}$	
$\phi(\vec{r})$	x
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-\left(kx - 1\right)\left(kx + 1\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2 xy$
$\nabla^2\phi(\vec{r})$	$k^2 x \left(k^2 r^2 - 4\right)$

Table 4: Orbital expressions HOOrbitals : 1, 0. Factor $e^{-\frac{1}{2}k^2 r^2}$ is omitted.

$\phi_3 \to \phi_{0,2}$	
$\phi(\vec{r})$	$2k^2 y^2 - 1$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2 x \left(2k^2 y^2 - 1\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2 y \left(2k^2 y^2 - 5\right)$
$\nabla^2\phi(\vec{r})$	$k^2 \left(k^2 r^2 - 6\right)\left(2k^2 y^2 - 1\right)$

Table 5: Orbital expressions HOOrbitals : 0, 2. Factor $e^{-\frac{1}{2}k^2 r^2}$ is omitted.

$\phi_4 \to \phi_{1,1}$	
$\phi(\vec{r})$	xy
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-y\left(kx - 1\right)\left(kx + 1\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-x\left(ky - 1\right)\left(ky + 1\right)$
$\nabla^2\phi(\vec{r})$	$k^2 xy \left(k^2 r^2 - 6\right)$

Table 6: Orbital expressions HOOrbitals : 1, 1. Factor $e^{-\frac{1}{2}k^2 r^2}$ is omitted.

$\phi_5 \to \phi_{2,0}$	
$\phi(\vec{r})$	$2k^2x^2 - 1$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2x\left(2k^2x^2 - 5\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2y\left(2k^2x^2 - 1\right)$
$\nabla^2\phi(\vec{r})$	$k^2\left(k^2r^2 - 6\right)\left(2k^2x^2 - 1\right)$

Table 7: Orbital expressions HOOrbitals : 2, 0. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_6 \to \phi_{0,3}$	
$\phi(\vec{r})$	$y\left(2k^2y^2 - 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2y^2 - 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-2k^4y^4 + 9k^2y^2 - 3$
$\nabla^2\phi(\vec{r})$	$k^2y\left(k^2r^2 - 8\right)\left(2k^2y^2 - 3\right)$

Table 8: Orbital expressions HOOrbitals : 0, 3. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_7 \to \phi_{1,2}$	
$\phi(\vec{r})$	$x\left(2k^2y^2 - 1\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-\left(kx - 1\right)\left(kx + 1\right)\left(2k^2y^2 - 1\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2y^2 - 5\right)$
$\nabla^2\phi(\vec{r})$	$k^2x\left(k^2r^2 - 8\right)\left(2k^2y^2 - 1\right)$

Table 9: Orbital expressions HOOrbitals : 1, 2. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_8 \to \phi_{2,1}$	
$\phi(\vec{r})$	$y\left(2k^2x^2 - 1\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2x^2 - 5\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-\left(ky - 1\right)\left(ky + 1\right)\left(2k^2x^2 - 1\right)$
$\nabla^2\phi(\vec{r})$	$k^2y\left(k^2r^2 - 8\right)\left(2k^2x^2 - 1\right)$

Table 10: Orbital expressions HOOrbitals : 2, 1. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_9 \to \phi_{3,0}$	
$\phi(\vec{r})$	$x\left(2k^2x^2 - 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-2k^4x^4 + 9k^2x^2 - 3$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2x^2 - 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2x\left(k^2r^2 - 8\right)\left(2k^2x^2 - 3\right)$

Table 11: Orbital expressions HOOrbitals : 3, 0. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{10} \to \phi_{0,4}$	
$\phi(\vec{r})$	$4k^4y^4 - 12k^2y^2 + 3$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2x\left(4k^4y^4 - 12k^2y^2 + 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2y\left(4k^4y^4 - 28k^2y^2 + 27\right)$
$\nabla^2\phi(\vec{r})$	$k^2\left(k^2r^2 - 10\right)\left(4k^4y^4 - 12k^2y^2 + 3\right)$

Table 12: Orbital expressions HOOrbitals : 0, 4. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{11} \to \phi_{1,3}$	
$\phi(\vec{r})$	$xy\left(2k^2y^2 - 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-y\left(kx - 1\right)\left(kx + 1\right)\left(2k^2y^2 - 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-x\left(2k^4y^4 - 9k^2y^2 + 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2xy\left(k^2r^2 - 10\right)\left(2k^2y^2 - 3\right)$

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

$\phi_{12} \to \phi_{2,2}$	
$\phi(\vec{r})$	$\left(2k^2x^2 - 1\right)\left(2k^2y^2 - 1\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2x\left(2k^2x^2 - 5\right)\left(2k^2y^2 - 1\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2y\left(2k^2x^2 - 1\right)\left(2k^2y^2 - 5\right)$
$\nabla^2\phi(\vec{r})$	$k^2\left(k^2r^2 - 10\right)\left(2k^2x^2 - 1\right)\left(2k^2y^2 - 1\right)$

Table 14: Orbital expressions HOOrbitals : 2, 2. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{13} \to \phi_{3,1}$	
$\phi(\vec{r})$	$xy\left(2k^2x^2 - 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-y\left(2k^4x^4 - 9k^2x^2 + 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-x\left(ky - 1\right)\left(ky + 1\right)\left(2k^2x^2 - 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2xy\left(k^2r^2 - 10\right)\left(2k^2x^2 - 3\right)$

Table 15: Orbital expressions HOOrbitals : 3, 1. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{14} \to \phi_{4,0}$	
$\phi(\vec{r})$	$4k^4x^4 - 12k^2x^2 + 3$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2x\left(4k^4x^4 - 28k^2x^2 + 27\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2y\left(4k^4x^4 - 12k^2x^2 + 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2\left(k^2r^2 - 10\right)\left(4k^4x^4 - 12k^2x^2 + 3\right)$

Table 16: Orbital expressions HOOrbitals : 4, 0. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{15} \to \phi_{0,5}$	
$\phi(\vec{r})$	$y\left(4k^4y^4 - 20k^2y^2 + 15\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(4k^4y^4 - 20k^2y^2 + 15\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-4k^6y^6 + 40k^4y^4 - 75k^2y^2 + 15$
$\nabla^2\phi(\vec{r})$	$k^2y\left(k^2r^2 - 12\right)\left(4k^4y^4 - 20k^2y^2 + 15\right)$

Table 17: Orbital expressions HOOrbitals : 0, 5. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{16} \to \phi_{1,4}$	
$\phi(\vec{r})$	$x\left(4k^4y^4 - 12k^2y^2 + 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-\left(kx - 1\right)\left(kx + 1\right)\left(4k^4y^4 - 12k^2y^2 + 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(4k^4y^4 - 28k^2y^2 + 27\right)$
$\nabla^2\phi(\vec{r})$	$k^2x\left(k^2r^2 - 12\right)\left(4k^4y^4 - 12k^2y^2 + 3\right)$

Table 18: Orbital expressions HOOrbitals : 1, 4. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{17} \to \phi_{2,3}$	
$\phi(\vec{r})$	$y\left(2k^2x^2 - 1\right)\left(2k^2y^2 - 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2x^2 - 5\right)\left(2k^2y^2 - 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-\left(2k^2x^2 - 1\right)\left(2k^4y^4 - 9k^2y^2 + 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2y\left(k^2r^2 - 12\right)\left(2k^2x^2 - 1\right)\left(2k^2y^2 - 3\right)$

Table 19: Orbital expressions HOOrbitals : 2, 3. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{18} \to \phi_{3,2}$	
$\phi(\vec{r})$	$x\left(2k^2x^2 - 3\right)\left(2k^2y^2 - 1\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-\left(2k^2y^2 - 1\right)\left(2k^4x^4 - 9k^2x^2 + 3\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(2k^2x^2 - 3\right)\left(2k^2y^2 - 5\right)$
$\nabla^2\phi(\vec{r})$	$k^2x\left(k^2r^2 - 12\right)\left(2k^2x^2 - 3\right)\left(2k^2y^2 - 1\right)$

Table 20: Orbital expressions HOOrbitals : 3, 2. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{19} \to \phi_{4,1}$	
$\phi(\vec{r})$	$y\left(4k^4x^4 - 12k^2x^2 + 3\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(4k^4x^4 - 28k^2x^2 + 27\right)$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-\left(ky - 1\right)\left(ky + 1\right)\left(4k^4x^4 - 12k^2x^2 + 3\right)$
$\nabla^2\phi(\vec{r})$	$k^2y\left(k^2r^2 - 12\right)\left(4k^4x^4 - 12k^2x^2 + 3\right)$

Table 21: Orbital expressions HOOrbitals : 4, 1. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.

$\phi_{20} \to \phi_{5,0}$	
$\phi(\vec{r})$	$x\left(4k^4x^4 - 20k^2x^2 + 15\right)$
$\vec{i} \cdot \nabla\phi(\vec{r})$	$-4k^6x^6 + 40k^4x^4 - 75k^2x^2 + 15$
$\vec{j} \cdot \nabla\phi(\vec{r})$	$-k^2xy\left(4k^4x^4 - 20k^2x^2 + 15\right)$
$\nabla^2\phi(\vec{r})$	$k^2x\left(k^2r^2 - 12\right)\left(4k^4x^4 - 20k^2x^2 + 15\right)$

Table 22: Orbital expressions HOOrbitals : 5, 0. Factor $e^{-\frac{1}{2}k^2r^2}$ is omitted.