

## 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  $k = \sqrt{(\omega\alpha)}$ , with  $\omega$  being the oscillator frequency and  $\alpha$  being the variational parameter.

$H_0(kx)$	1
$H_1(kx)$	$2kx$
$H_2(kx)$	$4k^2x^2 - 2$
$H_3(kx)$	$8k^3x^3 - 12kx$
$H_4(kx)$	$16k^4x^4 - 48k^2x^2 + 12$
$H_5(kx)$	$32k^5x^5 - 160k^3x^3 + 120kx$
$H_6(kx)$	$64k^6x^6 - 480k^4x^4 + 720k^2x^2 - 120$
$H_0(ky)$	1
$H_1(ky)$	$2ky$
$H_2(ky)$	$4k^2y^2 - 2$
$H_3(ky)$	$8k^3y^3 - 12ky$
$H_4(ky)$	$16k^4y^4 - 48k^2y^2 + 12$
$H_5(ky)$	$32k^5y^5 - 160k^3y^3 + 120ky$
$H_6(ky)$	$64k^6y^6 - 480k^4y^4 + 720k^2y^2 - 120$

Table 1: Hermite polynomials used to construct orbital functions

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

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

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

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

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

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

$\phi_3 \rightarrow \phi_{0,2}$	
$\phi(\vec{r})$	$4k^2 y^2 - 2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2k^2 x (2k^2 y^2 - 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2k^2 y (2k^2 y^2 - 5)$
$\nabla^2 \phi(\vec{r})$	$2k^2 (k^2 r^2 - 6) (2k^2 y^2 - 1)$

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

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

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

$\phi_5 \rightarrow \phi_{2,0}$	
$\phi(\vec{r})$	$4k^2x^2 - 2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2k^2x(2k^2x^2 - 5)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2k^2y(2k^2x^2 - 1)$
$\nabla^2 \phi(\vec{r})$	$2k^2(k^2r^2 - 6)(2k^2x^2 - 1)$

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

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

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

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

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

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

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

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

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

$\phi_{10} \rightarrow \phi_{0,4}$	
$\phi(\vec{r})$	$16k^4y^4 - 48k^2y^2 + 12$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-4k^2x(4k^4y^4 - 12k^2y^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-4k^2y(4k^4y^4 - 28k^2y^2 + 27)$
$\nabla^2 \phi(\vec{r})$	$4k^2(k^2r^2 - 10)(4k^4y^4 - 12k^2y^2 + 3)$

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

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

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

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

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

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

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

$\phi_{14} \rightarrow \phi_{4,0}$	
$\phi(\vec{r})$	$16k^4x^4 - 48k^2x^2 + 12$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-4k^2x(4k^4x^4 - 28k^2x^2 + 27)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-4k^2y(4k^4x^4 - 12k^2x^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$4k^2(k^2r^2 - 10)(4k^4x^4 - 12k^2x^2 + 3)$

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

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

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

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

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

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

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

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

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

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

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

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

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

$\phi_{21} \rightarrow \phi_{0,6}$	
$\phi(\vec{r})$	$64k^6y^6 - 480k^4y^4 + 720k^2y^2 - 120$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-8k^2x(8k^6y^6 - 60k^4y^4 + 90k^2y^2 - 15)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-8k^2y(8k^6y^6 - 108k^4y^4 + 330k^2y^2 - 195)$
$\nabla^2 \phi(\vec{r})$	$8k^2(k^2r^2 - 14)(8k^6y^6 - 60k^4y^4 + 90k^2y^2 - 15)$

Table 23: Orbital expressions HOOorbitals : 0, 6. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{22} \rightarrow \phi_{1,5}$	
$\phi(\vec{r})$	$xy(4k^4y^4 - 20k^2y^2 + 15)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-y(kx - 1)(kx + 1)(4k^4y^4 - 20k^2y^2 + 15)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-x(4k^6y^6 - 40k^4y^4 + 75k^2y^2 - 15)$
$\nabla^2 \phi(\vec{r})$	$k^2xy(k^2r^2 - 14)(4k^4y^4 - 20k^2y^2 + 15)$

Table 24: Orbital expressions HOOorbitals : 1, 5. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{23} \rightarrow \phi_{2,4}$	
$\phi(\vec{r})$	$(2k^2x^2 - 1)(4k^4y^4 - 12k^2y^2 + 3)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-k^2x(2k^2x^2 - 5)(4k^4y^4 - 12k^2y^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-k^2y(2k^2x^2 - 1)(4k^4y^4 - 28k^2y^2 + 27)$
$\nabla^2 \phi(\vec{r})$	$k^2(k^2r^2 - 14)(2k^2x^2 - 1)(4k^4y^4 - 12k^2y^2 + 3)$

Table 25: Orbital expressions HOOorbitals : 2, 4. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{24} \rightarrow \phi_{3,3}$	
$\phi(\vec{r})$	$xy(2k^2x^2 - 3)(2k^2y^2 - 3)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-y(2k^2y^2 - 3)(2k^4x^4 - 9k^2x^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-x(2k^2x^2 - 3)(2k^4y^4 - 9k^2y^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$k^2xy(k^2r^2 - 14)(2k^2x^2 - 3)(2k^2y^2 - 3)$

Table 26: Orbital expressions HOOorbitals : 3, 3. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{25} \rightarrow \phi_{4,2}$	
$\phi(\vec{r})$	$(2k^2y^2 - 1)(4k^4x^4 - 12k^2x^2 + 3)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-k^2x(2k^2y^2 - 1)(4k^4x^4 - 28k^2x^2 + 27)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-k^2y(2k^2y^2 - 5)(4k^4x^4 - 12k^2x^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$k^2(k^2r^2 - 14)(2k^2y^2 - 1)(4k^4x^4 - 12k^2x^2 + 3)$

Table 27: Orbital expressions HOOorbitals : 4, 2. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{26} \rightarrow \phi_{5,1}$	
$\phi(\vec{r})$	$xy(4k^4x^4 - 20k^2x^2 + 15)$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-y(4k^6x^6 - 40k^4x^4 + 75k^2x^2 - 15)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-x(ky - 1)(ky + 1)(4k^4x^4 - 20k^2x^2 + 15)$
$\nabla^2 \phi(\vec{r})$	$k^2xy(k^2r^2 - 14)(4k^4x^4 - 20k^2x^2 + 15)$

Table 28: Orbital expressions HOOorbitals : 5, 1. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.

$\phi_{27} \rightarrow \phi_{6,0}$	
$\phi(\vec{r})$	$64k^6x^6 - 480k^4x^4 + 720k^2x^2 - 120$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-8k^2x(8k^6x^6 - 108k^4x^4 + 330k^2x^2 - 195)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-8k^2y(8k^6x^6 - 60k^4x^4 + 90k^2x^2 - 15)$
$\nabla^2 \phi(\vec{r})$	$8k^2(k^2r^2 - 14)(8k^6x^6 - 60k^4x^4 + 90k^2x^2 - 15)$

Table 29: Orbital expressions HOOorbitals : 6, 0. Factor  $e^{-\frac{1}{2}k^2r^2}$  is omitted.