

angular momentum algebra

$$\vec{J} = \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix} \text{ where } J_i^\dagger = J_i \text{ and } [J_1, J_2] = iJ_3 \text{ (cyclic)}$$

orthonormal eigensystem

$$\begin{aligned} \vec{J}^2 |j, m\rangle &= j(j+1) |j, m\rangle & j \in \{0, 1/2, 1, 3/2, 2, \dots\} \\ J_3 |j, m\rangle &= m |j, m\rangle & m \in \{-j, -j+1, \dots, j\} \end{aligned}$$

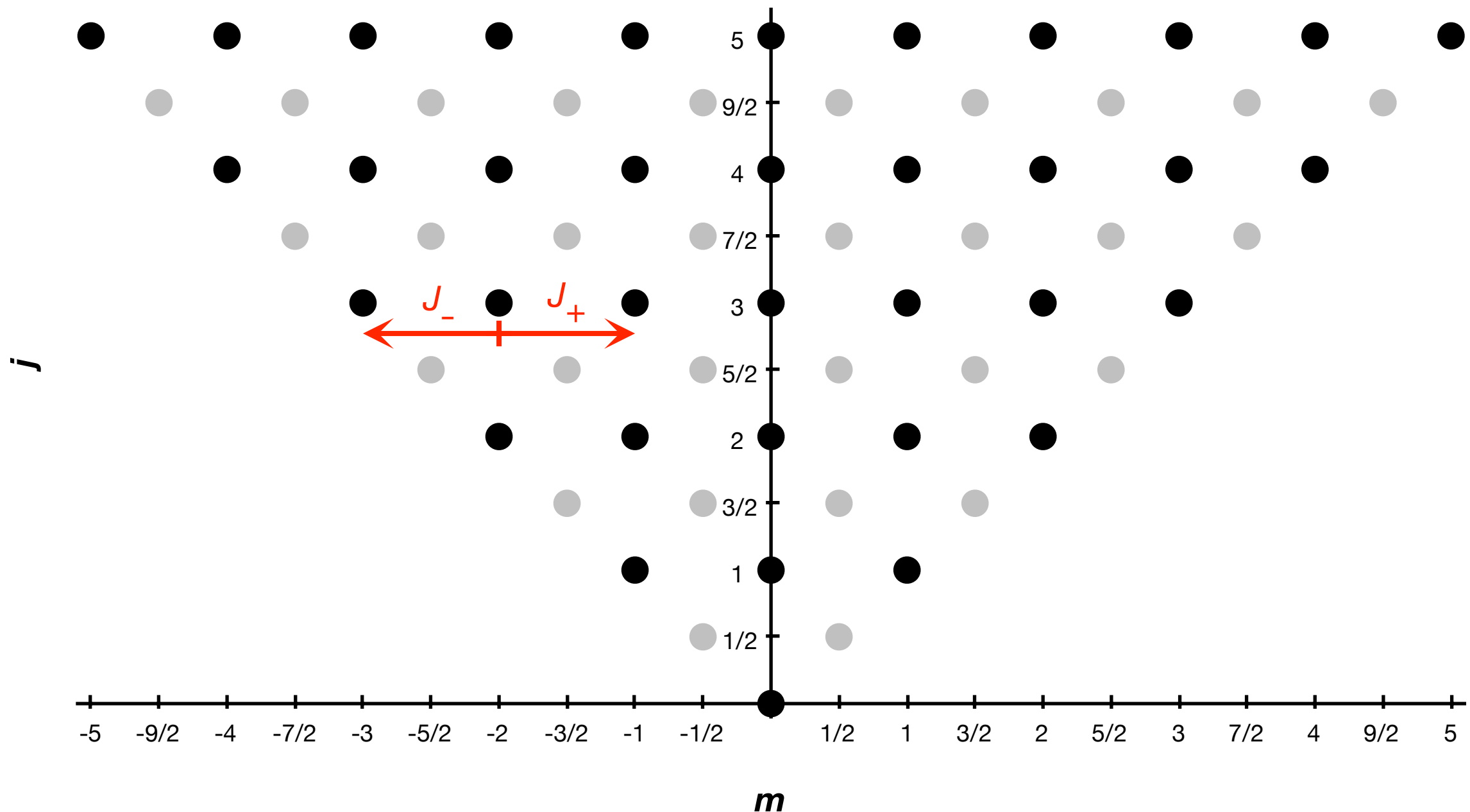
ladder operators $J_\pm = J_1 \pm iJ_2$

$$J_\pm |j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle$$

Condon-Shortley phase convention

angular momentum states

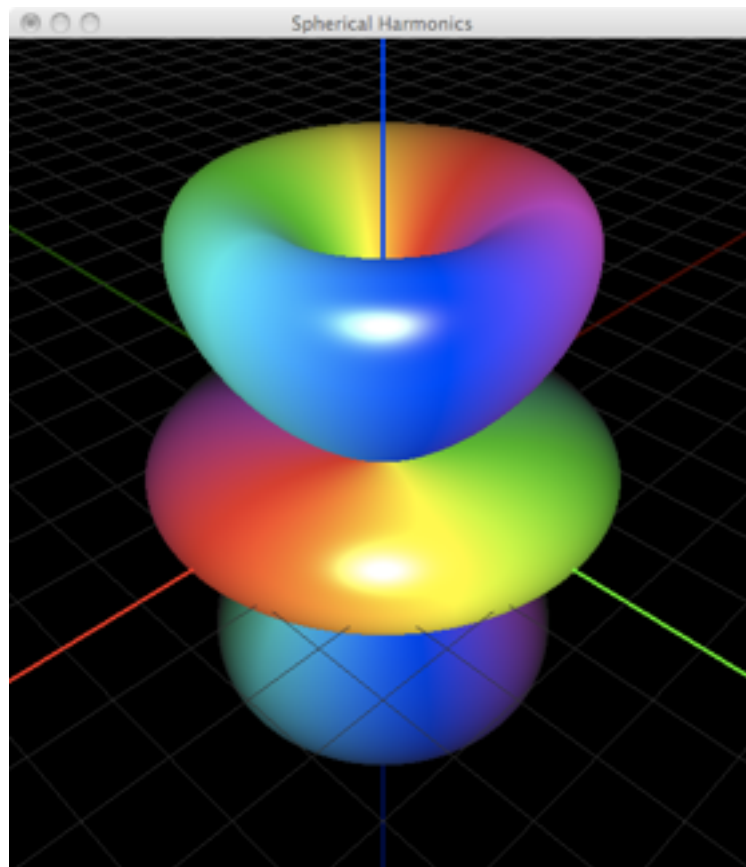
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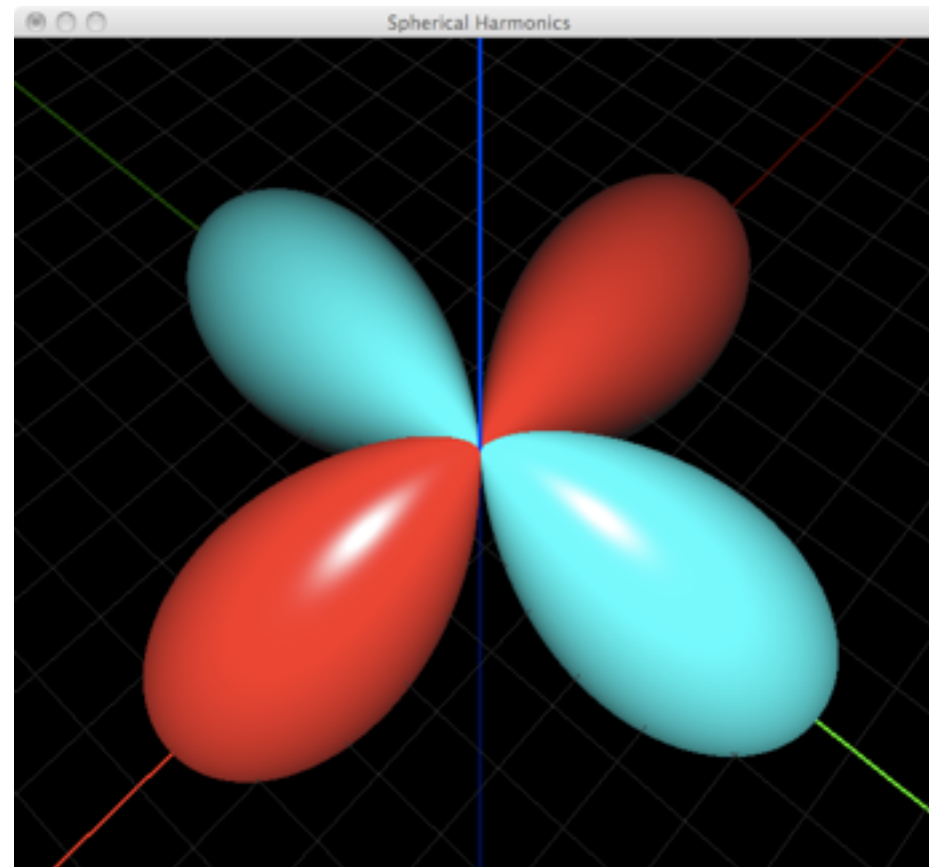
Visualizing Complex Functions using GPUs

Jülich Supercomputing Centre Guest Student Programme 2012

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$Y_{3,1}$

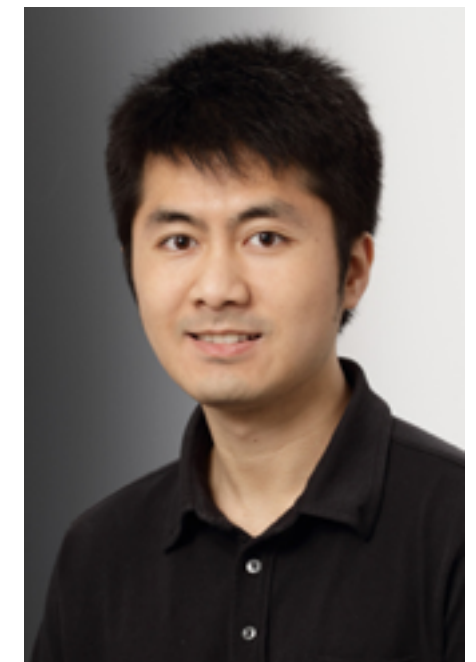
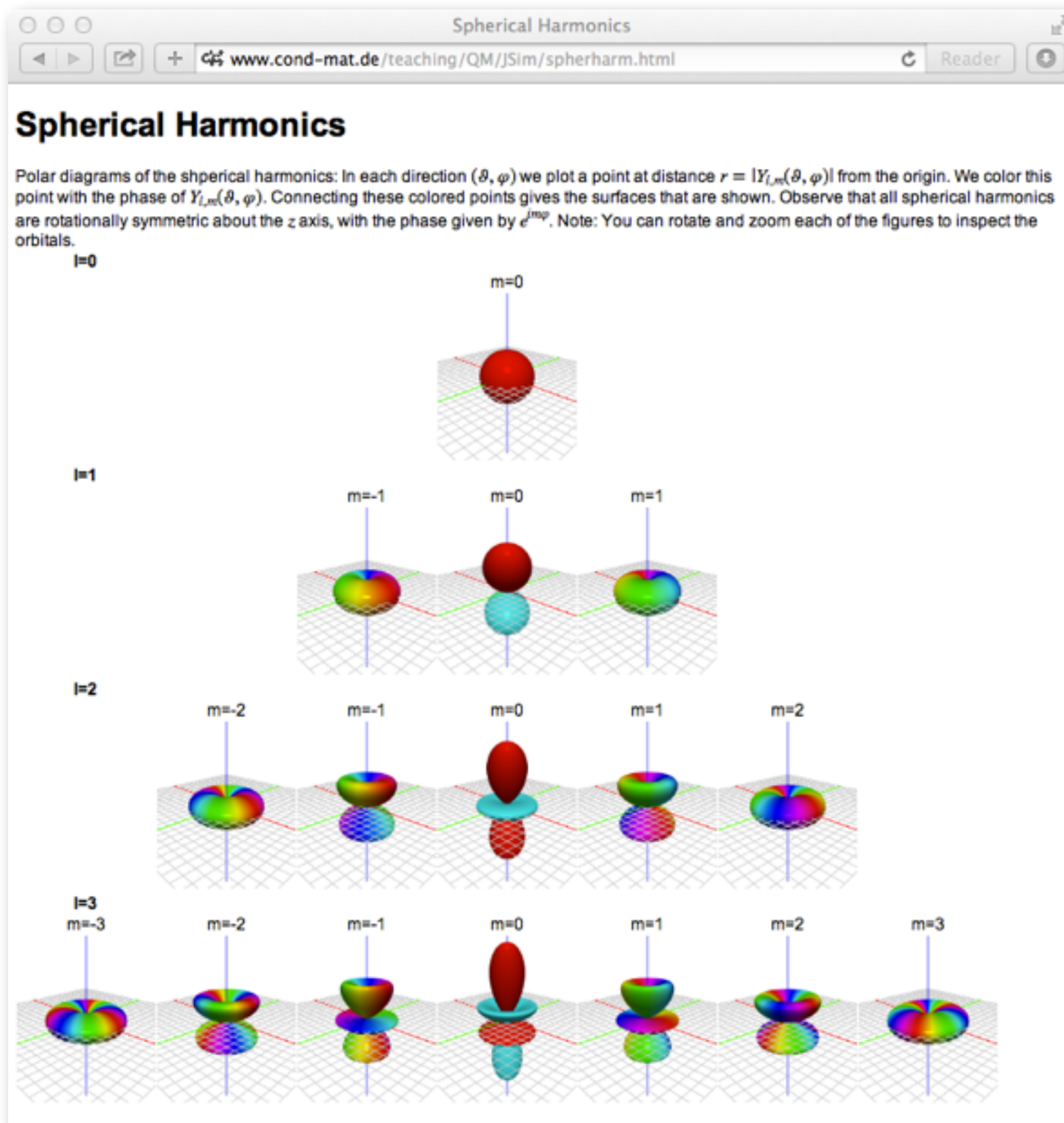


$d_{x^2-y^2}$



Khaldoon
Ghanem

interactive web page



Qian Zhang

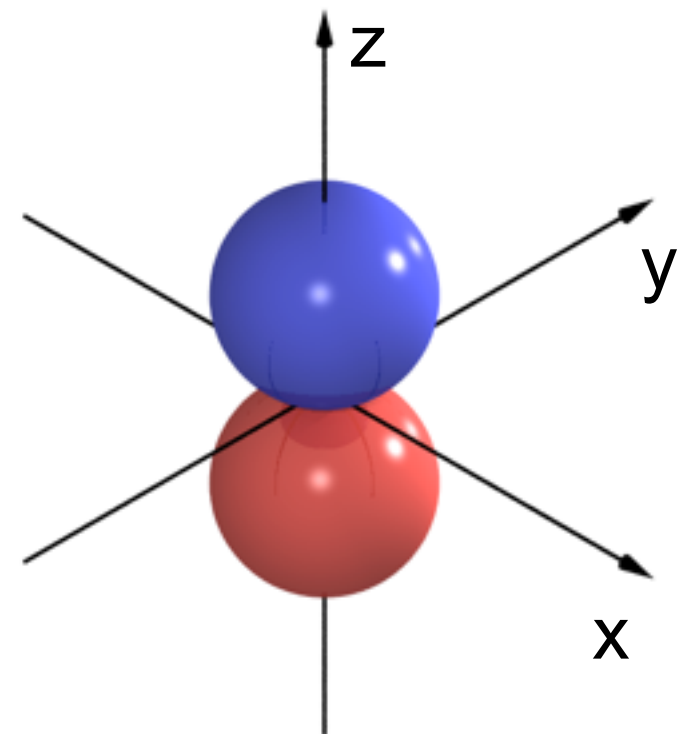
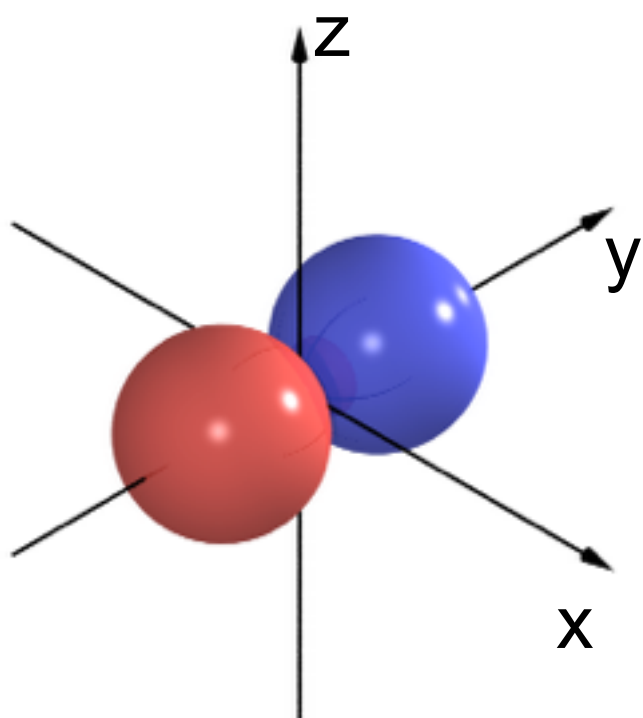
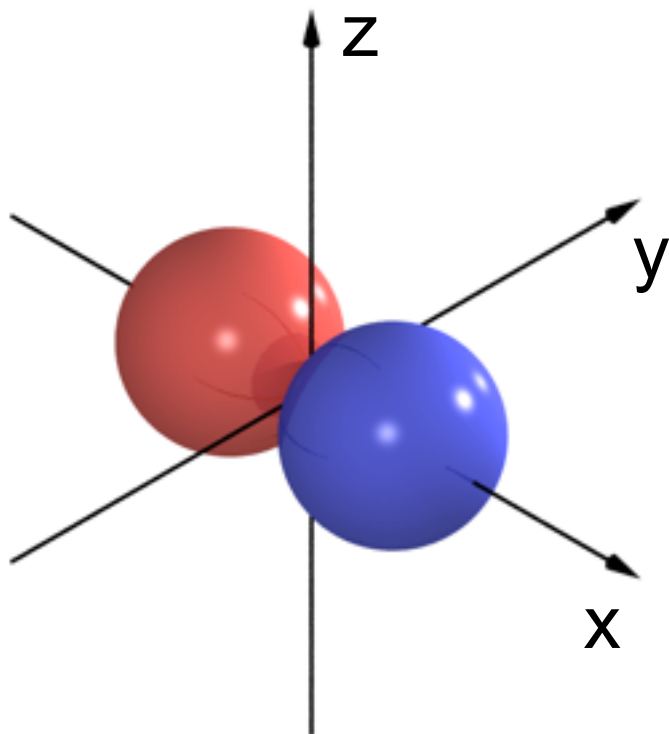
p-orbitals (*l*=1)

real orbitals

$$p_z = Y_{1,0}$$

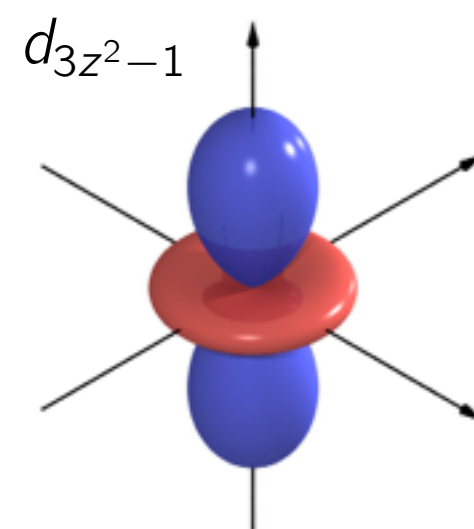
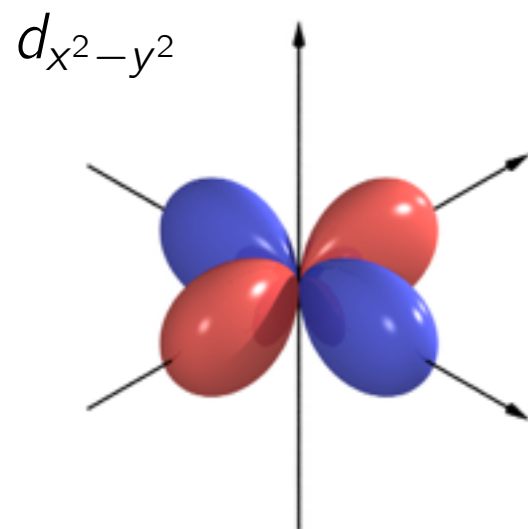
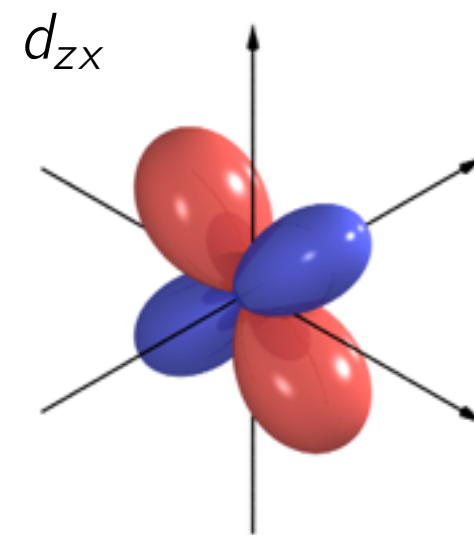
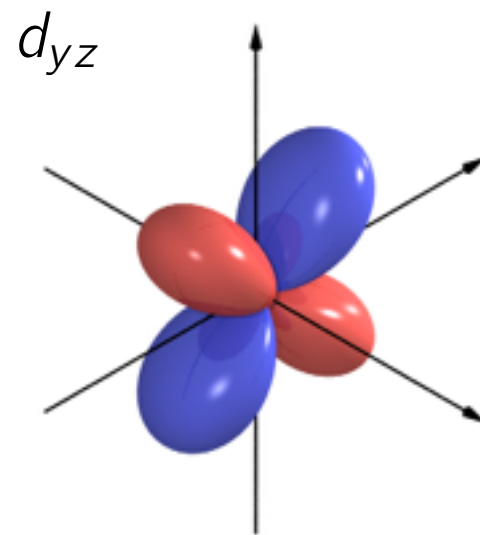
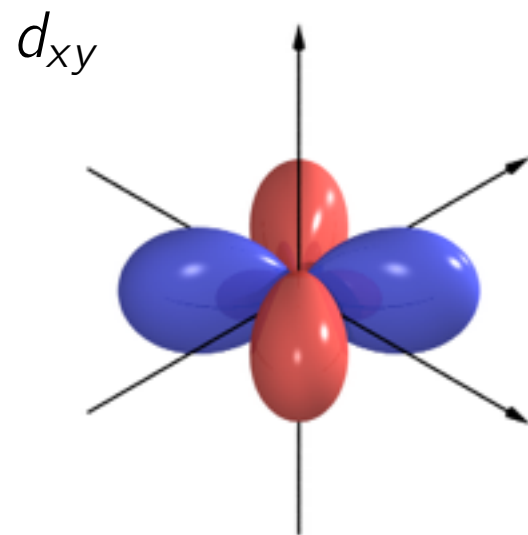
$$p_x = \sqrt{\frac{1}{2}}(Y_{1,-1} - Y_{1,1})$$

$$p_y = \sqrt{\frac{1}{2}}i(Y_{1,-1} + Y_{1,1})$$



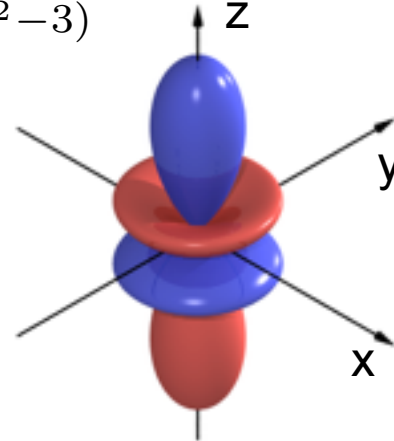
d-orbitals (*l*=2)

d_{3z^2-1}	$Y_{2,0}$	$\sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$
d_{zx}	$\sqrt{\frac{1}{2}} (Y_{2,-1} - Y_{2,1})$	$\sqrt{\frac{15}{16\pi}} \sin 2\theta \cos \phi$
d_{yz}	$\sqrt{\frac{1}{2}} i (Y_{2,-1} + Y_{2,1})$	$\sqrt{\frac{15}{16\pi}} \sin 2\theta \sin \phi$
d_{xy}	$\sqrt{\frac{1}{2}} i (Y_{2,-2} - Y_{2,2})$	$\sqrt{\frac{15}{16\pi}} \sin^2 \theta \cos \phi$
$d_{x^2-y^2}$	$\sqrt{\frac{1}{2}} (Y_{2,-2} + Y_{2,2})$	$\sqrt{\frac{15}{16\pi}} \sin^2 \theta \sin \phi$

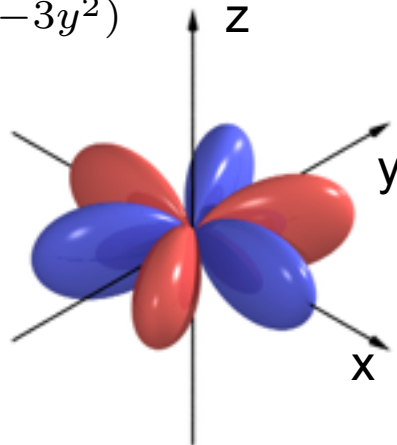


f-orbitals

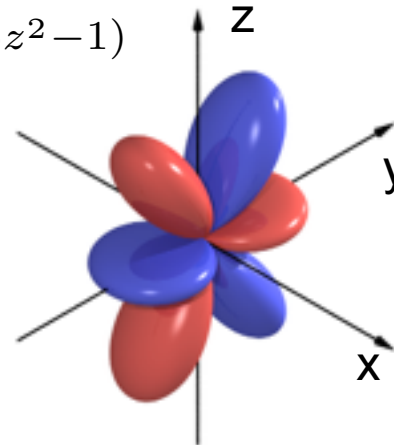
$$f_z(5z^2 - 3)$$



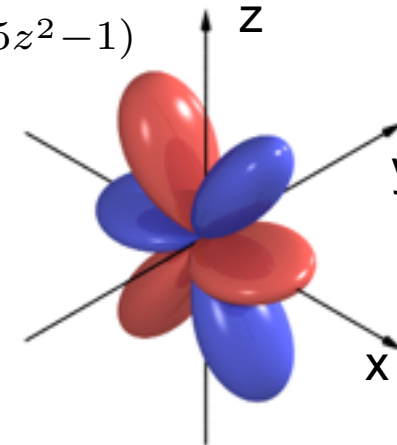
$$f_x(x^2 - 3y^2)$$



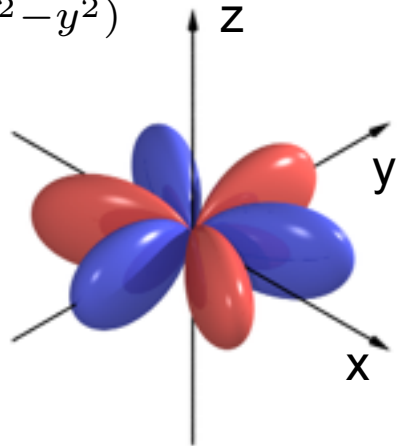
$$f_y(5z^2 - 1)$$



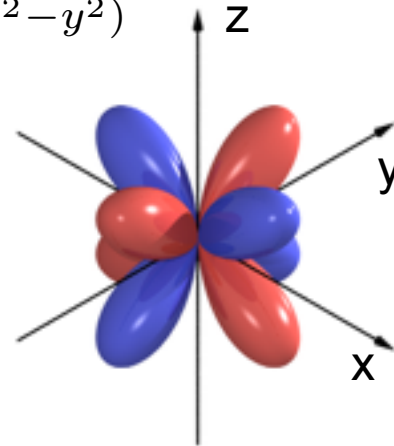
$$f_x(5z^2 - 1)$$



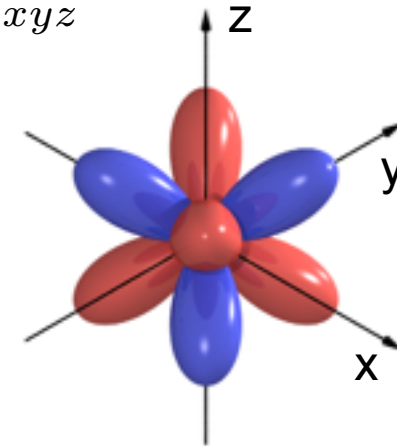
$$f_y(3x^2 - y^2)$$



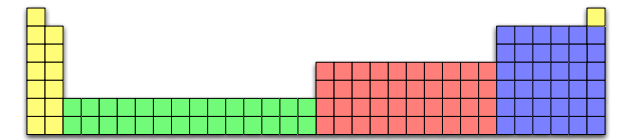
$$f_z(x^2 - y^2)$$



$$f_{xyz}$$



Periodic Table



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	● Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	●● Lr	Rf	Db	Sg	Bh	Hs	Mt									

● La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
●● Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

The diagram shows a simplified periodic table layout. It consists of several colored blocks: a yellow block on the far left (alkali and alkaline earth metals), a green block in the middle (transition metals), a red block on the right (main group elements), and a blue block on the far right (noble gases). The blocks are arranged in a way that shows their relative positions in the periodic table.

The diagram illustrates the arrangement of atomic orbitals in a periodic table format. The orbitals are color-coded and labeled as follows:

- Yellow (s orbitals):** 1s, 2s, 3s, 4s, 5s, 6s, 7s. The 6s orbital contains one electron (represented by a black dot), and the 7s orbital contains two electrons (represented by two black dots).
- Red (d orbitals):** 3d, 4d, 5d, 6d. Each d subshell contains five orbitals, represented by five vertical lines.
- Blue (p orbitals):** 2p, 3p, 4p, 5p, 6p. Each p subshell contains three orbitals, represented by three vertical lines.
- Green (f orbitals):** 4f, 5f. Each f subshell contains seven orbitals, represented by seven vertical lines.

The diagram shows the increasing number of orbitals per subshell (1, 3, 5, 7) and the increasing energy levels. The 6s orbital is shown with one electron, and the 7s orbital is shown with two electrons. The 4f and 5f orbitals are shown below the main grid.