angular momentum algebra

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

orthonormal eigensystem

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

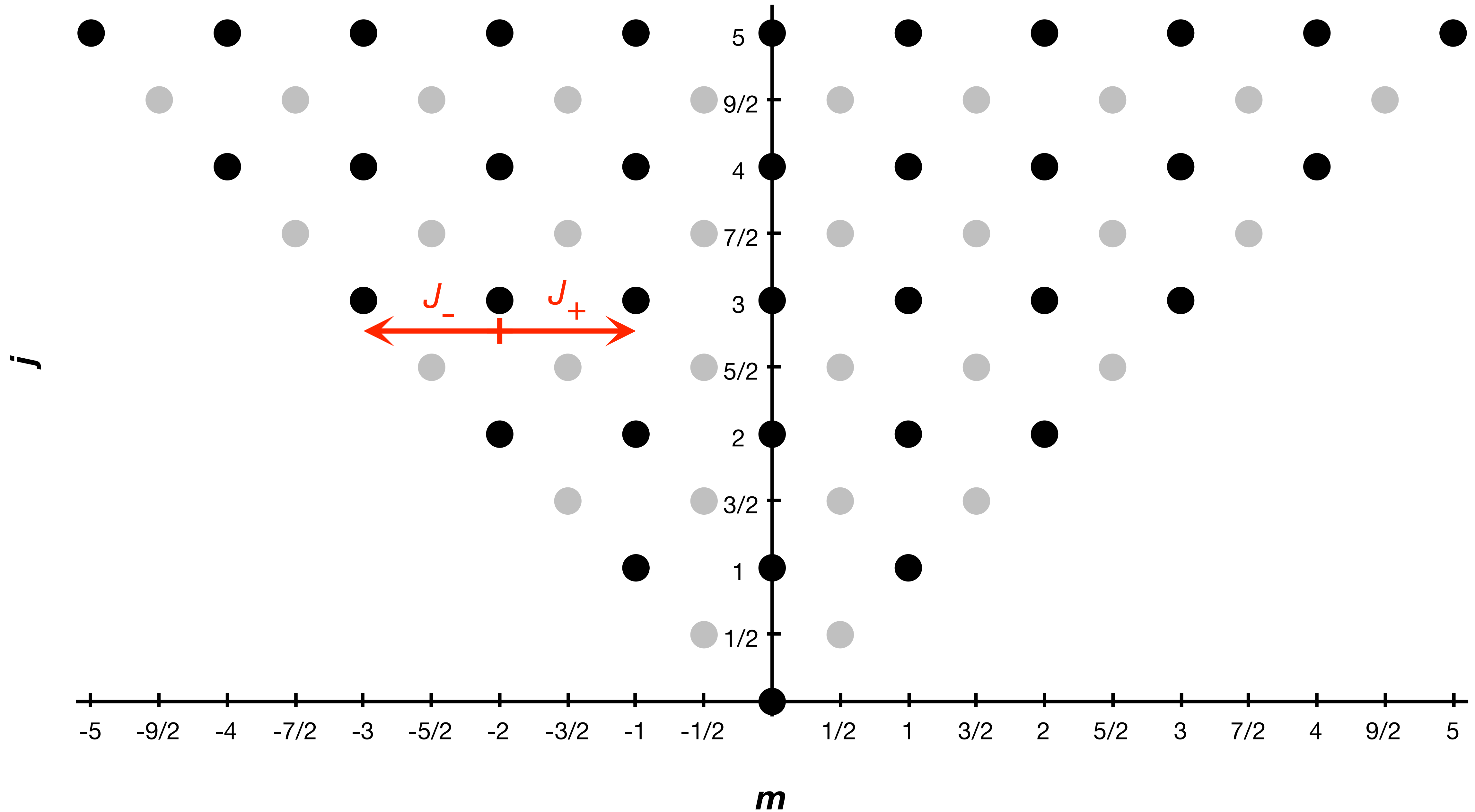
ladder operators $J_\pm = J_1 \pm i J_2$

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

Condon-Shortley phase convention

angular momentum states

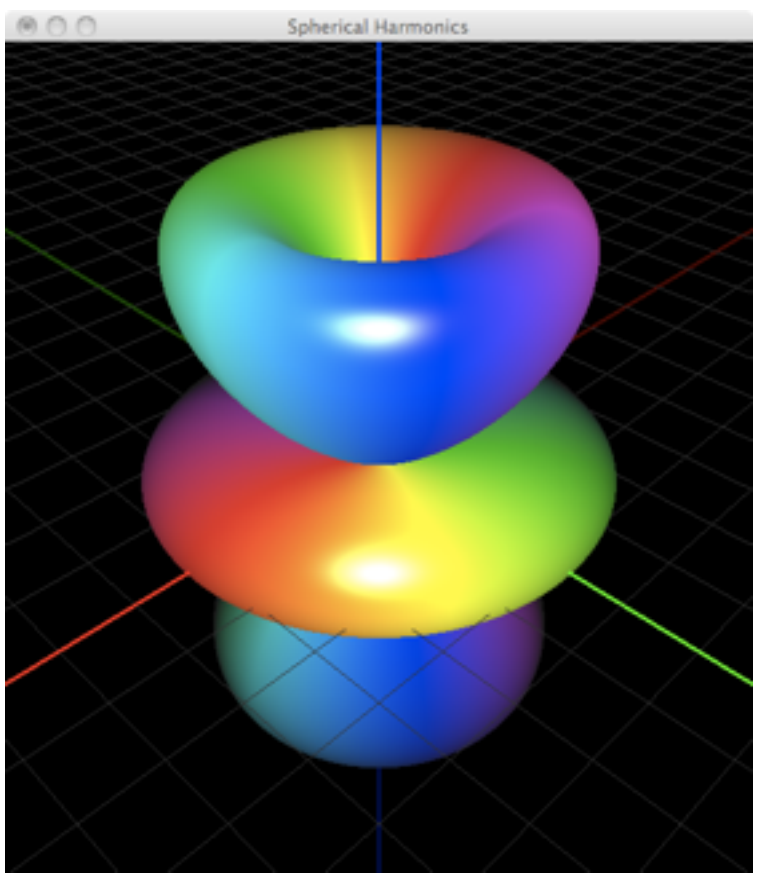
$$\vec{J}^2\,|j,m\rangle = j(j+1)\,|j,m\rangle$$
$$J_3\,|j,m\rangle = m\,|j,m\rangle$$



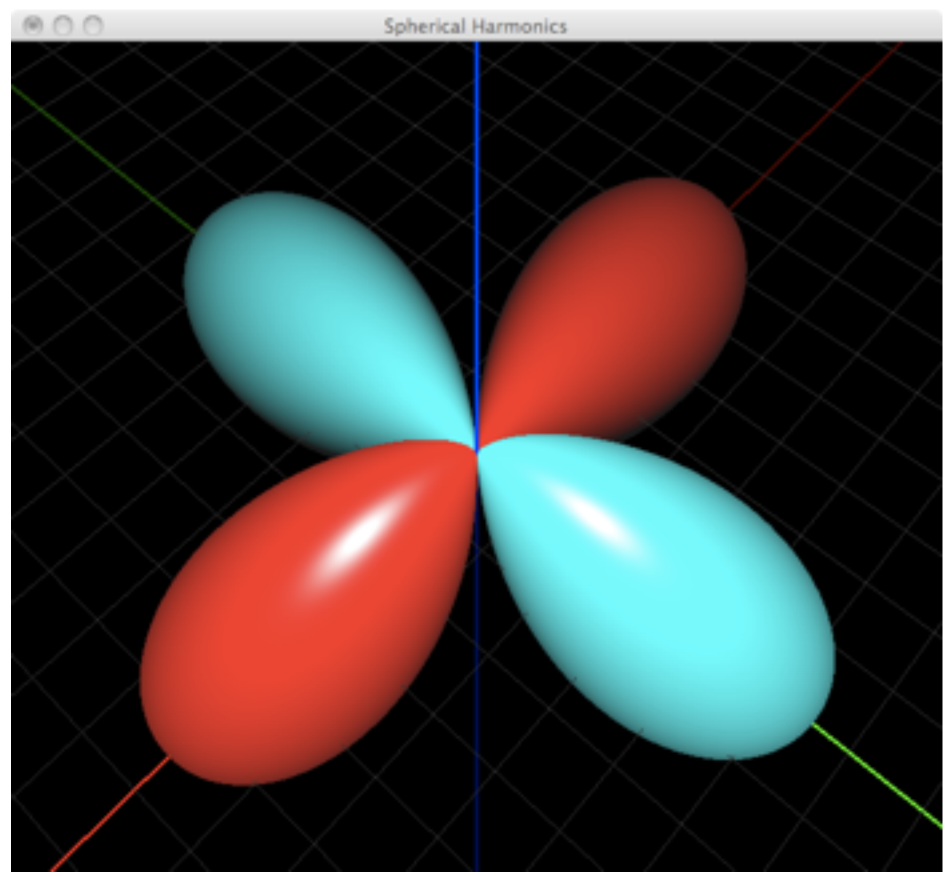
Visualizing Complex Functions using GPUs

Jülich Supercomputing Centre Guest Student Programme 2012

www.cond-mat.de/teaching/JSC/GSP12/



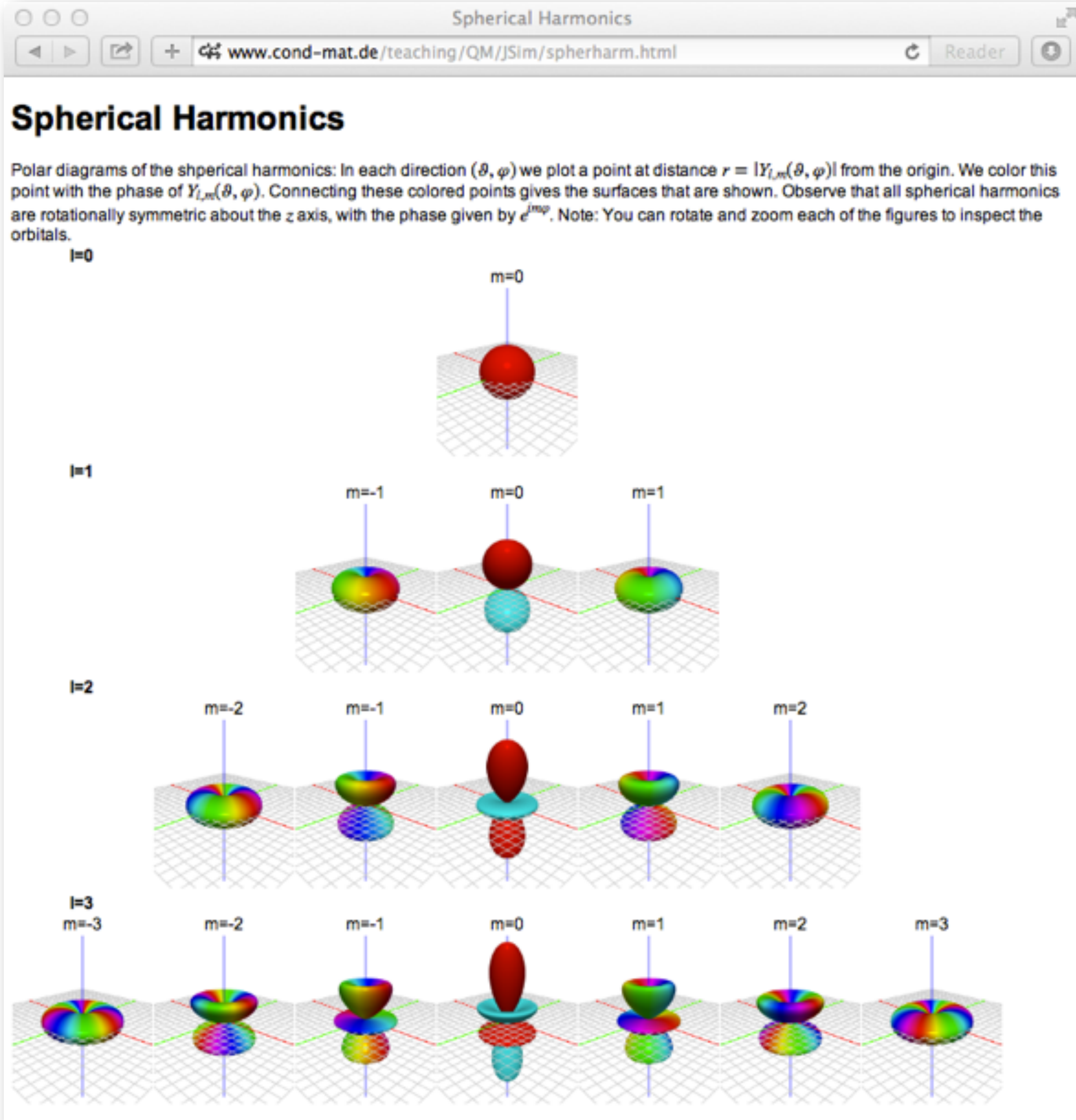
$Y_{3,1}$

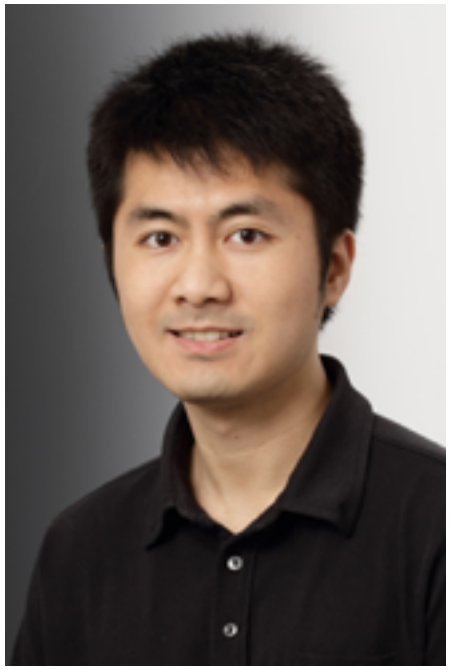


d_{x2-y2}

Khaldoon Ghanem

interactive web page



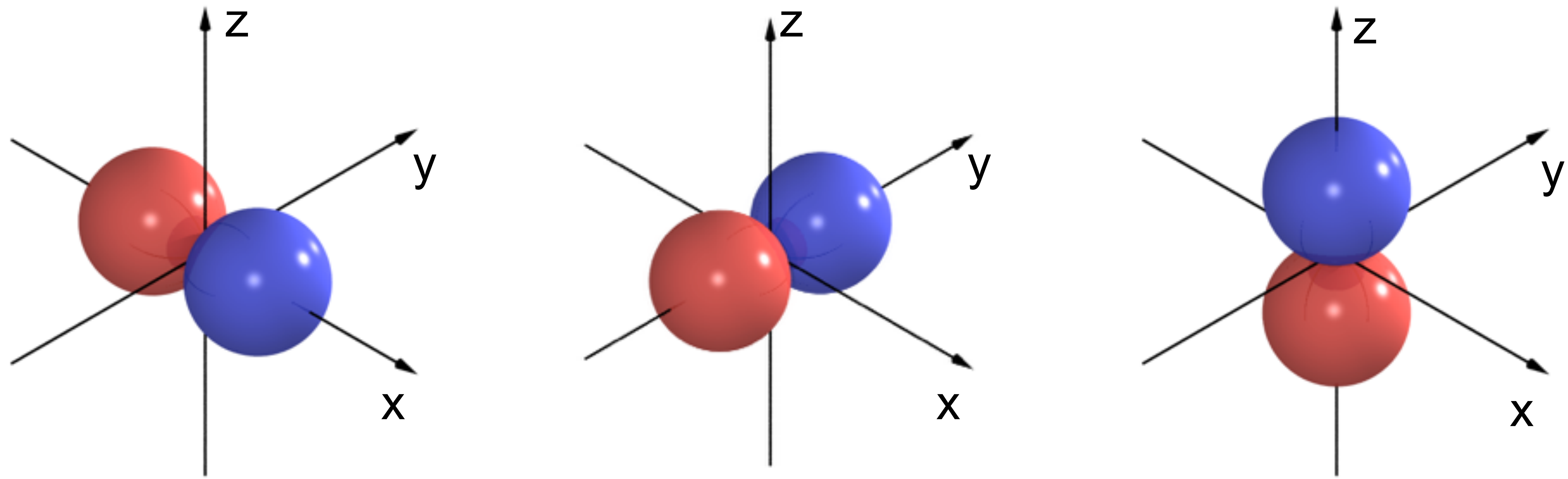


Qian Zhang

p-orbitals (l=1)

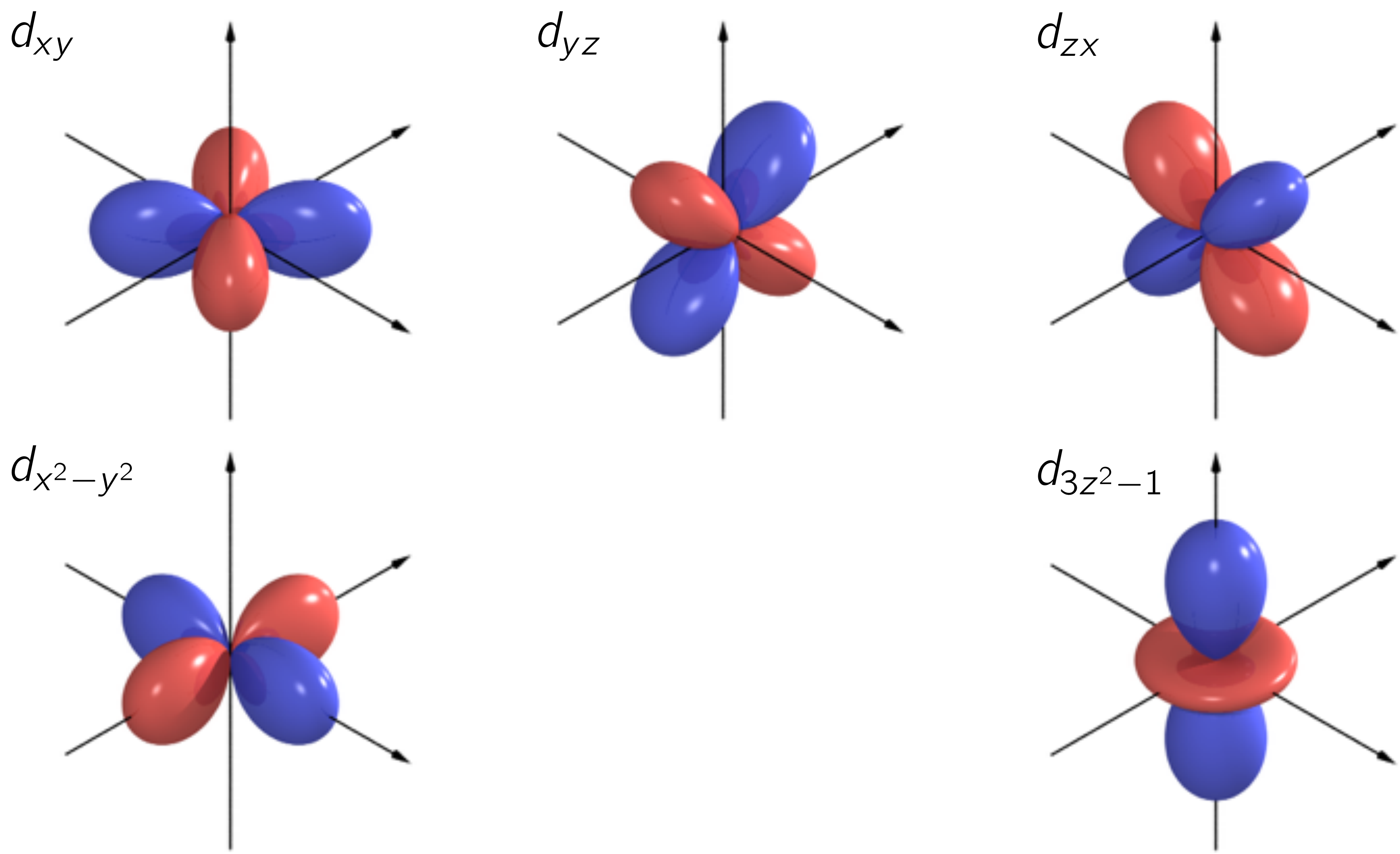
real orbitals

$$p_z = Y_{1,0}$$
$$p_x = \sqrt{\tfrac{1}{2}}(Y_{1,-1} - Y_{1,1})$$
$$p_y = \sqrt{\tfrac{1}{2}}\,i(Y_{1,-1} + Y_{1,1})$$



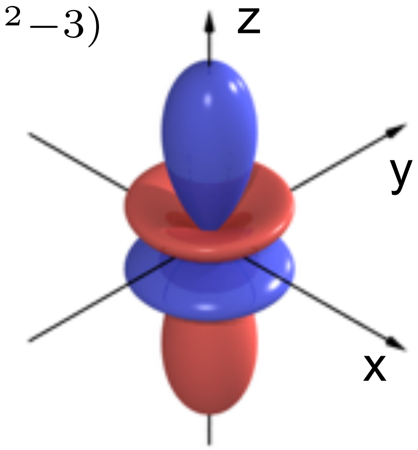
d-orbitals (l=2)

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}	$\sqrt{\frac{1}{2}}i(Y_{2,-2} - Y_{2,2})$	$\sqrt{\frac{15}{16\pi}}\ \sin^2\theta \cos\phi$
$d_{x^2-y^2}$	$\sqrt{\frac{1}{2}}(Y_{2,-2} + Y_{2,2})$	$\sqrt{\frac{15}{16\pi}}\ \sin^2\theta \sin\phi$

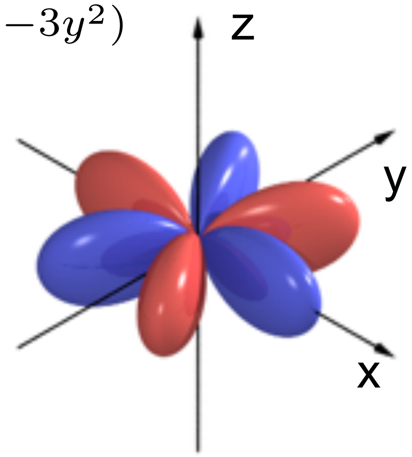


f-orbitals

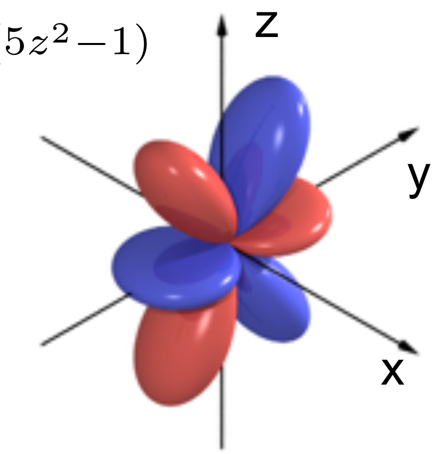
$f_{z(5z^2-3)}$



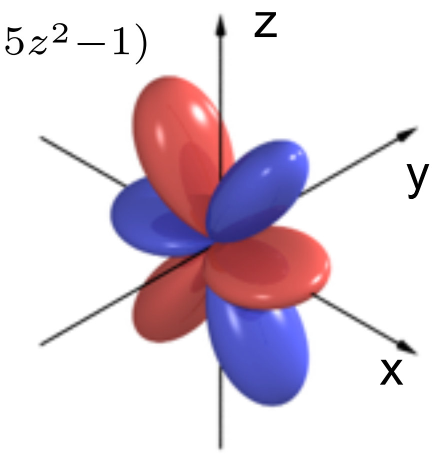
$f_{x(x^2-3y^2)}$



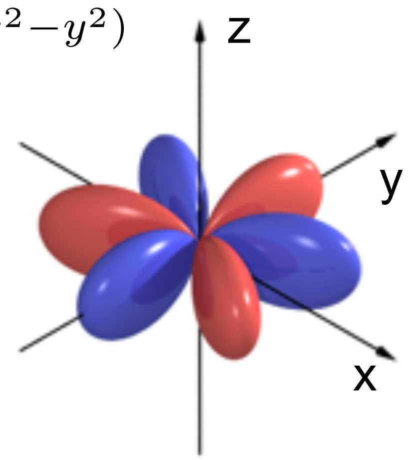
$f_{y(5z^2-1)}$



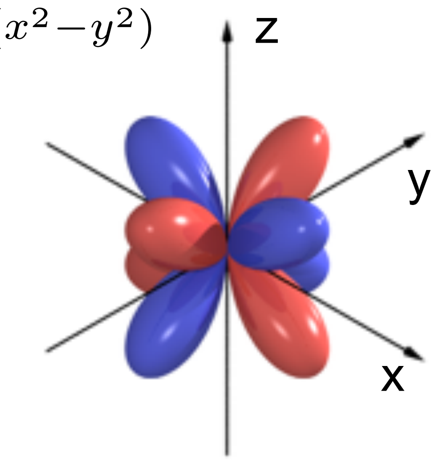
$f_{x(5z^2-1)}$



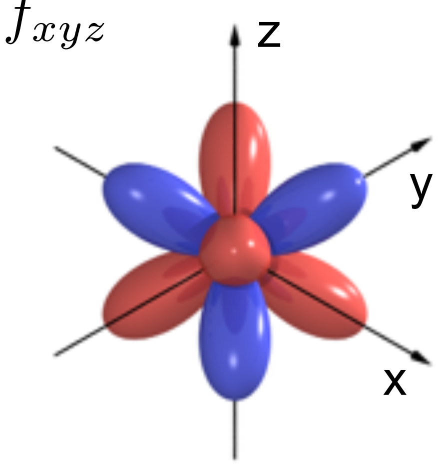
$f_{y(3x^2-y^2)}$



$f_{z(x^2-y^2)}$



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

Periodic Table