



Center for
Molecular
Modeling

Computational Materials Physics



Department of
Materials Science
and Engineering

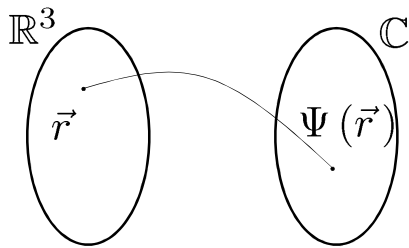
plotting wave functions and densities

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<http://molmod.ugent.be>
<http://www.ugent.be/ea/dmse/en>
my talks on Youtube: <http://goo.gl/P2b1Hs>

one-particle orbital with given spin

$$\Psi : \mathbb{R}^3 \rightarrow \mathbb{C} : \vec{r} \mapsto \Psi(\vec{r})$$

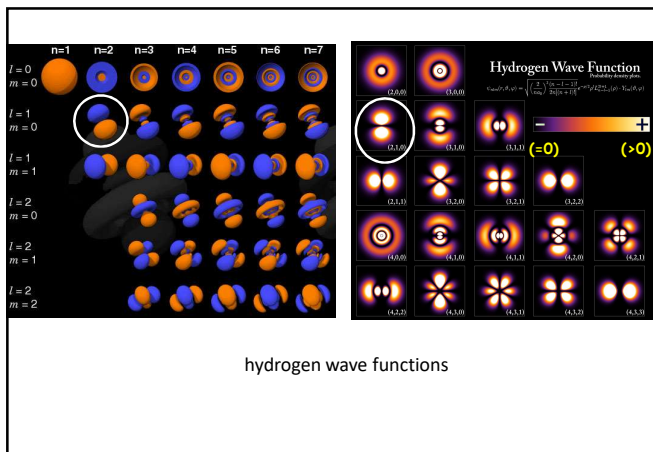


one-particle orbital with given spin

$$\Psi : \mathbb{R}^3 \rightarrow \mathbb{C} : \vec{r} \mapsto \Psi(\vec{r})$$

plot = 5 dimensions
reduction required

isosurfaces for $\text{Re}[\Psi]$ (with sign colour)
isosurfaces for $|\Psi|$
planar cut with colour scale for $\text{Re}[\Psi]$ or $|\Psi|$



one-particle density

$$\rho : \mathbb{R}^3 \rightarrow \mathbb{R} : \vec{r} \mapsto |\Psi(\vec{r})|^2 = \rho(\vec{r})$$

plot = 4 dimensions
reduction required

isosurfaces for ρ (always positive)
planar cut with colour scale ρ

