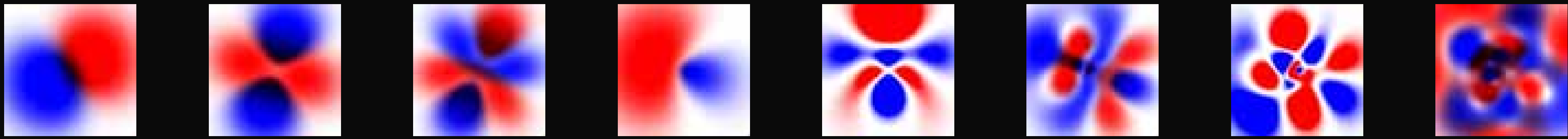


Waves ?

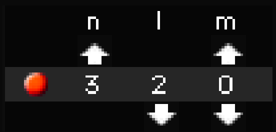
This software visualizes electrons in atoms. The so-called "orbitals" are 3-dimensional waves.

Waves ? - Yes, your teacher in school was definitely wrong when he said the electron was moving on a circle around the core. You've probably heard that light can be a wave **or** a particle. Electrons behave quite similarly. Quantum Mecanics is the theory which describes this wave-phenomena.

Orbitals is very easy to use and runs **real-time** on your Mac.

How to use it

When you start the Orbitals application, you will see the orbital |3,2,0> :



These three numbers are the Quantum Numbers of the orbital you are watching. The first number, "n" is the main quantum number, the energy level of the Atom. "l"describes the total angular momentum, and "m" is called angular momentum in z-direction.
But you don‘t have to learn all this. Just play and interact with your orbital by changing the numbers (click the little arrows). Rotate it by draging the mouse. Play with the zoom and the brightness. You'll get very nice real-time 3D visual effects.

Orbitals can calculate superpositions of up to 15 orbitals. This is an aproximation method which can describe atoms with more than one electron. Press the „+“-button to add another orbital. You can find some nice superpositions in the example-orbitals folder.

Have fun with it !

Behind the scenes

Orbital math:

The wave function |n,l,m> is the product of the radial and the two angular parts. You have to calculate two polynoms (P). The probability for a point is the square of the wave-function.

$$u = f_r \cdot f_\theta \cdot f_\phi \qquad p = |u|^2$$

$$f_r = r^l e^{-\frac{r}{n}} P_{(2\frac{r}{n})}$$

$$P[j] = \frac{(-1)^{j+1} ((n+l)!)^2}{(n-l-1-j)!\ (2l+1+j)!\ j!}$$

$$0 < j < n-l-1$$

$$f_\theta = (1 - E^2)^{\left|\frac{m}{2}\right|} P_{(E)}$$

1. $P_{(E)} := (E^2 - 1)^l$
2. differentiate P l times
3. $P_{(E)} := \frac{1}{2^l\ l!} P_{(E)}$
4. differentiate P $|m|$ times
5. $E := \cos(\theta)$

$$f_\phi = e^{im\phi} = \cos(m\phi) + i \sin(m\phi)$$

Orbitals calculates these wave-functions for 17x17x17 grid-points in space. Then it multiplies all 17 layers together to get the transparency effects. Bicubic interpolation is used to produce the final image.
Mouse-rotation is done by a quaternion matrix. You need this to rotate into the direction of the mouse movement.

Just email me if you have any questions or comments.

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