Mini-review of Electron Density Visualization

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Abstract

We describe both educational and research oriented examples of electronic density visualization with AViz. Several detailed cases are presented and the procedures for their preparation are described.

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1. Introduction

The wavelike nature of atoms, molecules and solids is a difficult concept for students to grasp. Since Rutherford we have known that atomic nuclei only take up a small part of atomic volumes, however the nuclei do not approach each other too closely because of the electronic density surrounding them. Electronic wavefunctions are known analytically for hydrogen and hydrogen-like atoms; but for other atoms and all molecules and multi-atom materials a numerical approach is needed.

There are many cases where the nature of the electronic wavefunctions needs to be understood. The first of these occurs in undergraduate quantum mechanics courses. Writing a complicated wavefunction including spherical harmonics does not immediately help students gain insight into atomic symmetry. When they are struggling with the particle-wave duality of atoms, orbital shapes can help gain insight. Explanation of different forms of inter-atomic bonding, with the canonical example being the structure of carbon allotropes wherein sp^2 and sp^3 wavefunctions give different geometric lattices, is much easier if the spatial nature can be shown.

Many materials require comphrehension of their electronic density to understand their structures. Nanotubes are the classic example, where the width of the nanotube wall has to be deduced in order to model, for example, vibrational behaviour. Bending and stretching properties are important and the bending of the tube is limited by the wall width.

2. Visualization

Electronic density is three dimensional, and varies in density as functions of distance from the nucleus and of angle. Two dimensional cuts and even succesive slices are not always helpful except for very simple uniform cylindrical
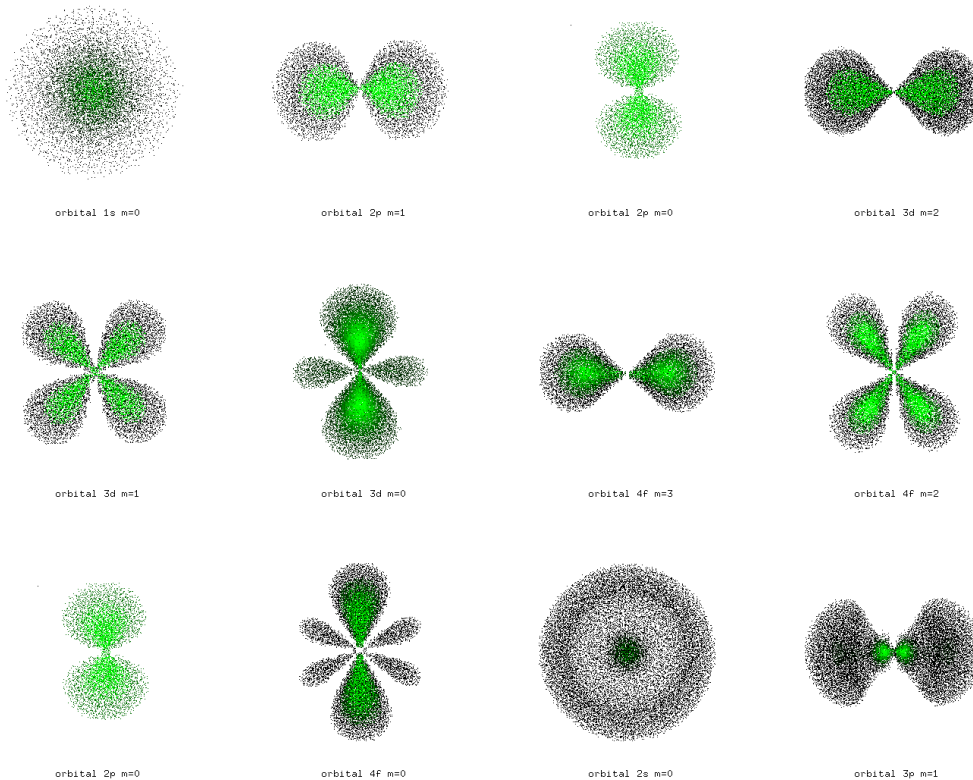
Figure 1. AViz dot visualizations of electronic density of states of an H atom.

cases. Visualization techniques such as rotation, zoom, and building up images layer-by-layer are helpful. Partial transparency also gives insight. Stereo vision is good; and stereo with limited cost can be important for educational use. All these techniques can be implemented in the public domain AViz (Atomistic Vizualization) package [1, 2], developed at the Technion and now part of the FP7 SimPhoNy project [3].

3. The educational hydrogen atom case

When students first meet hydrogen atom wavefunctions they often have difficulty grasping that s orbitals are symmetric in radius, r and angular states, p, d, f are not. 2D graphs cannot not show this. A beautiful old figure (1930s) of White [4] shows hydrogen atom wave functions, pictured by photographing spinning tops. The smoke rendering visualization technique can be used to show electronic density but this is usually done with white "smoke" [5]. When we were developing the AViz visualization package for atomistic simulation and discussing how to show electronic density we thought that perhaps, applying it off-label using the dot representation would work. We found that using an extensive color palette was very confusing, but binned color worked quite well.

The initial procedure was quite staightforward, as developd by Joey Fox [6, 7]:

- Use MATHEMATICA to express the analytical solutions for hydrogen atom wavefunctions, which are in spherical coordinates at a mesh of cartesian points.