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Visualization of electronic density

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ABSTRACT

The spatial volume occupied by an atom depends on its electronic density. Although this density can only be evaluated exactly for hydrogen-like atoms, there are many excellent algorithms and packages to calculate it numerically for other materials. Three-dimensional visualization of charge density is challenging, especially when several molecular/atomic levels are intertwined in space. In this paper, we explore several approaches to this, including the extension of an anaglyphic stereo visualization application based on the AViz package for hydrogen atoms and simple molecules to larger structures such as nanotubes. We will describe motivations and potential applications of these tools for answering interesting physical questions about nanotube properties.

1. Introduction and educational applications

The Computational Physics group at the Technion developed a desktop visualization code for their needs in Atomistic Visualization, called AViz, [1–3]. It is based on Mesa/OpenGL and Qt. Initially we modeled atoms as balls, spins as cones or vectors and quadrupolar molecules or liquid crystals or pores as cylinders. In a project motivated by educational use we invoked an "off-label" AViz implementation to illustrate the electronic probability density as calculated from the H atom analytic solution in a smoke rendering form [4], using dots to enable semi-transparency. The dot representation of AViz, originally created to enable quick selection of viewing angle etc. for atomistic samples, creates a translucent effect whereby the sample's interiors are visible. Combined with color and rotation it gives excellent insight into the nature of the different electronic states [5].

In order to draw the electronic density we (obviously) first need to calculate it. In brief, for the H atom one calculates the electronic density on a grid, and defines a box around each grid point. Dots are then drawn at randomly chosen points within each box at an average density equal to the local electronic density at the center of the box. Each of these points is given x, y and z coordinates and is drawn using the dot feature of AViz. The *.xyz* format is common to many molecular visualization packages, but its normally used to indicate atoms, not density points. For the hydrogen 2s case the datafiles contain some 50,000 points, rather larger than those typically used in atomic visualization, although since they are not solid spheres, the rendering time is reasonable. In the left frames of Fig. 1 we show the AViz visualization of the electronic density of the 2s state of the H atom in both grayscale and color. Three dimensional visualizations of hydrogen atom wavefunctions are very helpful for teaching Modern Physics or Quantum Mechanics classes. The concept of electronic density is hard to grasp. Animated gifs of these samples in rotation are found at [5] using binned color and have been found to be helpful to students [6].

Visualization of electronic density for atoms or small molecules is a bit different from volume visualization of, for example, fluid flow around an airplane wing because in the latter case there are one (or more) solid wings with fluid around, whereas in the atomic case we have one or many pinpoint nuclei and different electron orbitals for each. It is also different than water density in a cloud as electronic densities are more structured. Even the electronic density around a metal has a surface comprised of the inner conduction bands as a platform and a few additional free

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0010-4655/

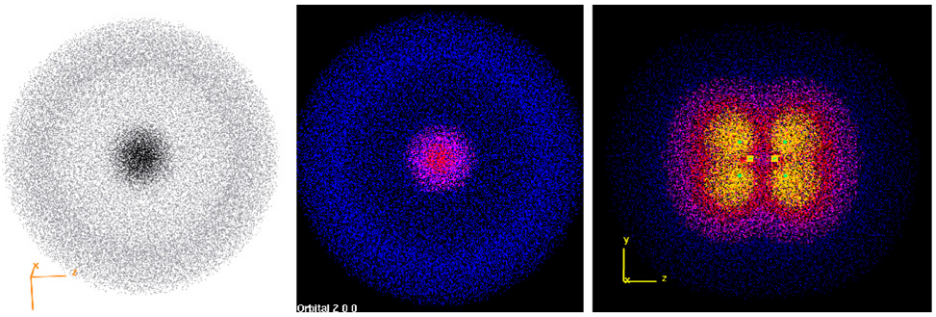

Fig. 1. AViz dot visualizations of the electronic density of the 2s state of an H atom in grayscale (left), and in color (center), and an ethylene molecule in color (right). The atoms in the ethylene are indicated by small squares, and the color scale of the density ranges from orange (most dense) through red and pink to blue (least dense) in all cases. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

electrons. As we will mention later on, there has been much study of atomic orbitals with techniques that visualize 2 dimensional cuts, or even sequential planes thereof. Covalent materials such as nanotubes are a bit different than surfaces of metals or even single atoms because one aims for semi-transparency in order to show depth and different layers of density. For our aim of actually measuring the thickness when the surface is curved, we really need to have a 3 dimensional space.

This paper includes detailed references to our codes, and these codes can all be found at [7] and in the CPC program library and server [8]. We provide details with some reference to the Technion's parallel multinode server, TAMNUN, which has the Redhat LINUX operating system and PBS queuing system, but have tested parts on non-parallel LINUX machines with interactive runs as well. The AViz used throughout is version 6.1, which has downloadable sources on [2], and continued development on GitHub [9]. It is currently available for several LINUX flavors, and under development for Windows. In the next section we discuss visualization for molecules and nanostructures, and in Section 3 we describe stereo visualization and binned color smoke rendering. This is followed by a section describing earlier nanotube visualizations, and in Section 5 we present general aspects of the calculations and visualizations. We devote Section 6 to details of the 3D charge density visualization, and in Section 7 some specifics for anaglyphic stereo. Section 8 covers some physics aspects.

2. Molecules and solids, especially nanostructures

A natural extension of electronic density visualization for single atoms is to molecules and simple nanostructures. In this area, experiment has advanced more quickly than simulation. We note that there are many quite standard implementations of smoke density approaches to surface electronic density simulating STM images, but most do not use color as well as concentration to indicate the density of their "smoke". Nor do they generally publish 3D images which can be rotated and sliced as AViz can, to peer inside the sample. In less transparent visualization some unique aspects of nanostructures may be overlooked.

Our extension of AViz applications aimed to visualize the electronic density resulting from simulations of larger molecules and solids in the same way. Initial studies [10] used a density functional theory approach with Slater-type orbitals (STO-3G) as implemented in GAMESS [11] to examine the electronic densities of simple molecules where there is no analytic solution. The graphical procedure is similar. In the right frame of Fig. 1 we show the colored electronic density of ethylene. Note that because the density is not shown with solid curves we can peer nicely into the sample. We have also been able to show methane molecules both with all orbitals and stripped of the lower densities, and have also explored specific orbitals [10,12,13].

Our next attempt at electronic density visualization was to periodically bounded samples, employing plane wave DFT calculations as implemented in the Vienna Ab Initio Simulation package VASP [14,15]. In preparation for the larger samples, we returned to some of the simple molecules with the VASP code. At that time we used slice visualization with VESTA [16], since dot visualization for many atom samples was limited by issues related to the large datafile size. Despite the VESTA solid visualization, rather than the 3D dot-smoke type, we confirmed that the main features agree. Note that VESTA images also include green in the color range, the early AViz ones only used a red–blue scale for better depth perception.

3. Stereo, binned color smoke rendering

The next stage in our visualization development was to move to 3D stereo. We selected an approach that has a long history, even predating GL. This old concept of anaglyphic stereo relies on two images, slightly displaced, and viewed on a regular screen/projector or poster [17] through colored glasses, or two squares of cellophane. Stereo Vision (SV) works by showing a different image to each eye, thus creating the illusion of a 3D image.

AViz 6.1 [2,18–20] has incorporated the possibility of SV, and although more than two colors are possible there remains some color washout, depending on color selection. The SV images generated by AViz, such as those in this paper, are best viewed using red–cyan anaglyphic glasses. The images in Fig. 2 show nanotube atoms at two different viewing angles in stereo.

In Fig. 3 we show (on the left) the electron density of an hydrogen atom in stereo. Improved colors for stereo for the H atom, as well as clearer instructions were given by Meital Kreif in [21,22]. Two examples are given in Fig. 3 (center) and (right), the former for the $n = 3, l = 1, m = 1$ orbital and the latter for the $n = 4, l = 3, m = 2$ orbital of the H atom. On the website [21] all images can be rotated to further aid in depth perception.

4. Motivation and preparation for studying the electronic density of nanotubes

A nanotube vibrates at a frequency that is a function of its width, length, tension, boundary conditions and for certain boundary conditions also of its type. A molecule placed on such a vibrating tube will change this frequency, enabling elucidation of the mass of the adsorbed molecule. The description of these systems with analytic models is limited in cases when both ends are not completely clamped, as occurs in the laboratory. The essential parameter for model analysis is the width of the nanotube wall, and it is the electronic cloud around the atomic nuclei that determines this.