Quantum Orbitals

Goal

To interpret correctly concepts such as "orbitals" and "electron clouds" often encountered in chemistry courses.

Introduction

Orbitals, electron clouds, shells, etc. are popular terms used in chemistry and other science courses. With quantum mechanics, we can understand details of how electrons behave in an atom and the meanings of these terms. In this tutorial, we will investigate quantum orbitals using computer simulations and see how orbitals and electronic clouds are related to wave functions.

A. 1S States of a Hydrogen Atom

In this section, you are exploring to see how much you know about the "s-shell" of a hydrogen atom. Work through the following questions **before using any simulations**.

A-1. In the space below, sketch to show the shape of a 1s orbit (ground state).

A-2. Based on your sketch, what can you tell about the behavior of an electron in the ground state?

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A-3. The sketches of orbitals often appear as three-dimensional spheres. For the 1s orbit, describe and explain the probability for an electron in the 1s state to exist

- inside the sphere

- on the sphere

- outside the sphere

A-4. Suppose we were to use a Y-Z plane to "slice" the s-shell, at different locations along the X-axis. Figure 1 illustrates the location of a "slice" in the X-Y plane. In the space below, sketch the resulting patterns of the cross-sections you expect to see at X equals 0, 1, 2, and 3.

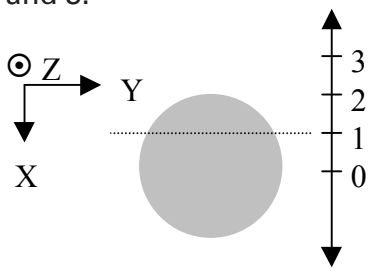


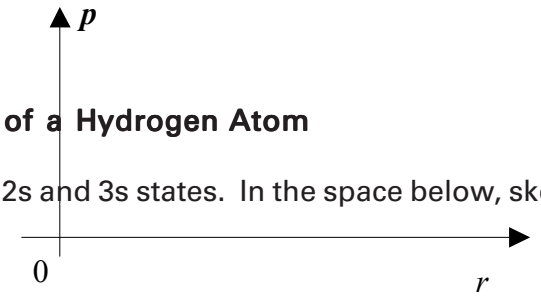
Figure 1: Example of taking a "slice" at X equals 1 from the perspective of the X-Y plane.

A-5. Explain how your sketches represent the probability of locating a 1s electron around the nucleus.

A-6. Based on your answer to the previous question, describe the probability of finding an electron in an s-state at different distances from the center (nucleus) of the atom.

A-7. On the graph provided, sketch the probability density of finding an s-state electron vs. the distance, *r*, from the center of the atom.

A-8. What is the relationship between the probability density plot and the wave function of the electron in a 1s state?



B. High Order s-states of a Hydrogen Atom

B-1. Now let's consider 2s and 3s states. In the space below, sketch the "shells" for 2s and 3s states.

B-2. Based on what you know about hydrogen atoms, describe the similarities and differences between the "shells" for 1s, 2s, and 3s states.

B-3. Obtain graphs from the instructor which show the radial part of the wave function for the 2s and 3s states. In the space below, sketch the probability density vs. r based on the radial part of the wave function.

B-4. Describe the probability of finding an electron in a 2s-state at different distances from the center (nucleus) of the atom.

B-5. Describe the probability of finding an electron in a 3s-state at different distances from the center of the atom.

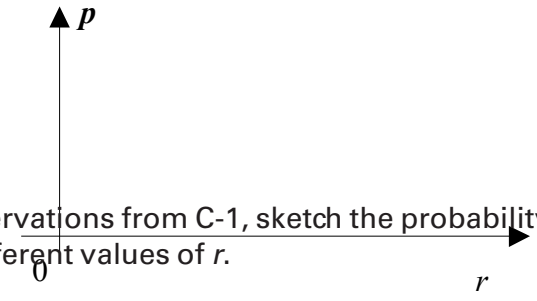
B-6. Suppose we also "slice" the "shells" of the 2s and 3s states in a similar manner to what we did in A-4. Based on the radial plots in B-3, predict and sketch the patterns of the cross-section at the four different X positions for both 2s and 3s states.

C. Computer Simulations

Now start the computer program *Atomic Explorer*. This simulation assists you in visualizing the cross-sectional slices of different atoms you have been mentally doing in the first two sections. Click on the *1s energy level* near the bottom left corner of the left window. In the right window, a cross-sectional slice should appear. You can change the position of the "slicing" plane by clicking on the axis to the left of the cube shown in the bottom of the right window. Try several different slicing positions and observe the patterns of the cross-sections of the s-orbit.

C-1. Now set the slicing plane to be in the Y-Z plane and change its position in the X direction to be approximate the four slices from question A-4. Sketch the patterns created by the simulation.

C-2. Compare your observations with the predictions you made and resolve any discrepancies.



C-3. Based on your observations from C-1, sketch the probability density of finding a 1s-state electron at different values of *r*.

C-4. In the program, choose *Radial Plot* from the *Display* menu. A pop-up window will display the radial part of the wave function. Sketch the wave function generated by the simulation.

C-5. Based on this radial plot, sketch the probability density of finding a 1s-state electron at different values of *r* and compare it to your sketch in C-3.

C-6. Now use the simulation to obtain cross-sections of the 2s and 3s orbitals (using the "slicing" settings described in A-4) and sketch the cross-sectional patterns generated.

C-7. Compare your observations with the predictions you made and resolve any discrepancies.

C-8. Describe how your observations are consistent with the graphs of the radial part of the wave functions you considered in question B-3.

C-9. Now choose *Isosurface* from the *Display* menu. This displays a three-dimensional surface representing an orbital. Using the 2s state as an example, explain how the orbitals, the isosurface, the wave function, the radial plot, and the probability of the electron being at different places around the nucleus are related.

D. Non-s-states of a Hydrogen Atom

For states other than s-states, the "shells" will have shapes that are angular-dependent. Thus, it is insufficient to use the radial plot to describe the orbits. To obtain a clearer picture of the structures of these states, we can use the "slicing" method to study different cross-sections.

D-1. Use the program to explore the 2p state. In the space below, sketch a few typical "slicing" patterns and explain the quantum interpretation that you can conclude from these patterns. (Explicitly address issues such as quantum wave function and the probability density of finding the electron in different locations around the nucleus.)

D-2. Now do the same thing with the 3d state.

E. Summary

As we have seen from this tutorial, the spheres used to represent quantum orbitals have quite complicated meanings. Write a summary of what you have learned and discuss how to relate this representation with the quantum wave function.