

# An Attempt to Construct an Isosurface Having Symmetry Elements

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Symmetry elements in various hydrogen atomic orbitals are summarized with respect to quantum numbers  $n$ ,  $l$  and  $m$ . The results are useful to improve the efficiency of drawing the isosurfaces of these orbitals.

**Keywords:** Isosurface, Computer graphics, Visualization, Atomic orbital, Symmetry operation

## 1 Introduction

An isosurface is a surface that represents points of a constant value, for example, temperature, pressure, density, and so on. Isosurfaces are displayed by computer graphics, and are used as visualization methods in many fields of chemistry. Orbital wavefunction, probability density, electron density and electrostatic potential have been visualized as isosurfaces [1–11]. The most promising method to draw isosurfaces has been reported as “marching cubes algorithm” [12]. Although the usefulness of the above algorithm has been established by many websites [13–15] and original papers [11, 12, 16], another method for the drawing of an isosurface of an atomic orbital is pursued in this paper with a novel attempt to use symmetry operations.

## 2 Volume visualization based on symmetries in atomic orbitals

The Schrödinger equation of an electron of a hydrogen atom is represented as follows.

$$\left[ -\frac{\hbar^2}{8\pi^2 m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{k_0 e^2}{r} \right] \chi = E \chi \quad (1)$$

where,  $\hbar$  is Planck’s constant,  $m$  is a mass of an electron,  $k_0$  is the electrostatic constant (Coulomb force constant),

$e$  is an elementary charge, and  $x, y, z$  are coordinates of an electron. The solutions,  $\chi$  of the equation (1) are called atomic orbital wavefunctions.

It turns out that each orbital is defined by three quantum numbers that are restricted to certain discrete values.

- (i) The principal quantum number,  $n = 1, 2, \dots$ , determines the energy  $E$  of the electron in the atom.
- (ii) The azimuthal quantum number,  $l = 0, 1, 2, \dots, n-1$ , determines the orbital angular momentum of the electron.
- (iii) The magnetic quantum number,  $m = 0, \pm 1, \dots, \pm l$  determines the amount of angular momentum of the electron around a particular axis.

Since the wavefunction  $\chi_{nlm}$  is a complex quantity where  $m \neq 0$ , it is transformed by the following linear combinations (2)–(3).

$$\chi_A = \frac{1}{\sqrt{2}} (\chi_{nlm} + \chi_{nl-m}) \quad (2)$$

$$\chi_B = \frac{1}{i\sqrt{2}} (\chi_{nlm} - \chi_{nl-m}) \quad (3)$$

The orbitals thus obtained are called 1s, 2s, 2p, 3s, 3p, 3d, …, where the numbers 1, 2, 3, …, correspond to the values of  $n$ , and the letters s, p, d, …, correspond to the values of  $l$ .

$l = 0, 1, 2, 3, 4, \dots$   
 $s, p, d, f, g, \dots$

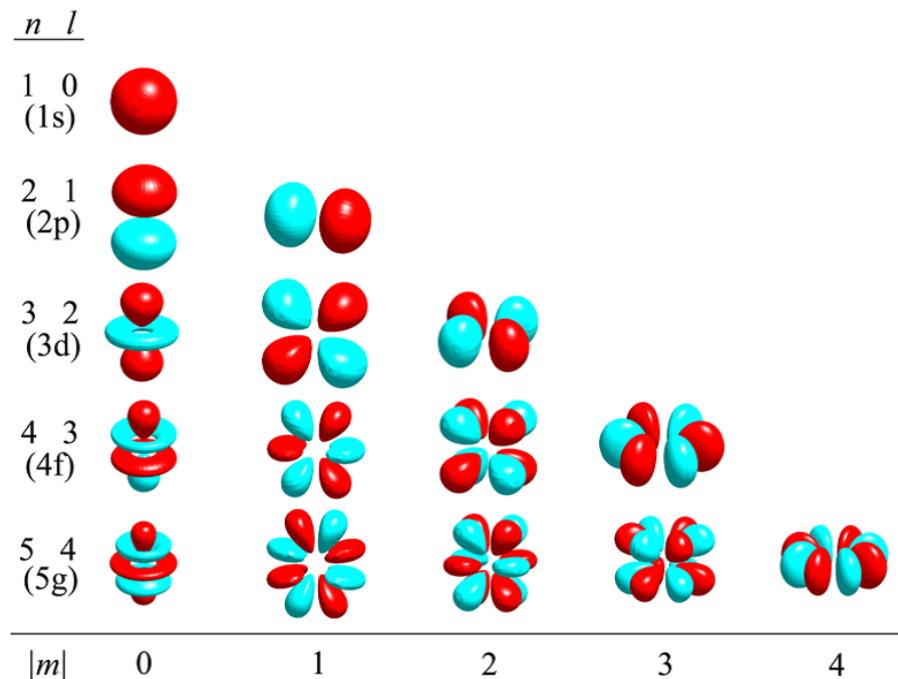


Figure 1. Isosurfaces of hydrogen atomic orbitals

The letters then run alphabetically, with the omission of i.

The shape of the isosurfaces of hydrogen atomic orbitals is shown in Figure 1. As the shapes of the orbitals represented by the equation (2) or (3) are identical, one of them is shown in Figure 1. These atomic orbitals have the following symmetry.

The 1s, 2s, 3s, ··· atomic orbitals, namely, the orbitals having the value of azimuthal quantum number  $l = 0$ , have spherical symmetry, in other words, have symmetry of  $C_\infty$  with respect to every axis including the origin.

The shortest way to draw the isosurface of 1s orbital,

$$\chi_{1s} = \frac{1}{\sqrt{\pi}} \exp(-r) \quad (4)$$

where,  $r = \sqrt{x^2 + y^2 + z^2}$ , is to calculate the function value of  $\chi_{1s}$  from  $r = 0$  to  $+\infty$  until the value reaches an appropriate constant  $a$ , for example,

$$\chi_{1s} = a = 0.001 \text{ au}^{-3/2} \quad (5)$$

and to give a sphere centered on the origin and having radius  $r$  that satisfies the equation (5).

In the case of  $\chi_{2s}$  orbital, the maximum number of such spheres having the constant value of  $\pm a$  is 4. The isosurfaces having the constant value of  $a = \pm 0.027 \text{ au}^{-3/2}$

are drawn as concentric spheres (a small sphere of  $a = +0.027 \text{ au}^{-3/2}$ , and a large sphere of  $a = -0.027 \text{ au}^{-3/2}$ ) as are shown in Figure 2.

A vertical line of  $r = 3.5 \text{ au}$  in Figure 2 left represents the distance from the origin to one of the 6 faces of the cube in Figure 2 right.

The atomic orbitals having the value of magnetic quantum number  $m = 0$  have cylindrical symmetry of  $C_\infty$  with respect to the Z axis ( $C_\infty^z$ ). When the value of the azimuthal quantum number  $l$  is even, the atomic orbital is symmetric with respect to  $\sigma(xy)$ , on the other hand, when  $l$  is odd, the orbital is antisymmetric with respect to  $\sigma(xy)$ .

For example, in order to draw the isosurfaces of  $\chi_{4f_{5,3-3z^2}}$  atomic orbital ( $n = 4$ ,  $l = 3$ ,  $m = 0$ ), we must obtain only two red lines in the first quadrant A and B in Figure 3. Antisymmetric operation with respect to XY plane and succeeding rotational operation with respect to Z axis gave a framework shown in Figure 4. Shading and smoothing procedure gave the isosurfaces represented in Figure 1.

When the value of the azimuthal quantum number  $l$  equals  $n-1$ , and the value of magnetic quantum number  $m$  equals  $+1$  or  $-1$ , the shape of the resulting orbitals  $\chi_{np_x}$  or  $\chi_{np_y}$  obtained by equation (2) or (3) is identical with the  $\chi_{np_z}$  atomic orbital ( $l = n-1$ ,  $m = 0$ ) because  $\chi_{np_x}$  orbital has a symmetry axis  $C_\infty^x$  and  $\chi_{np_y}$  has  $C_\infty^y$ .

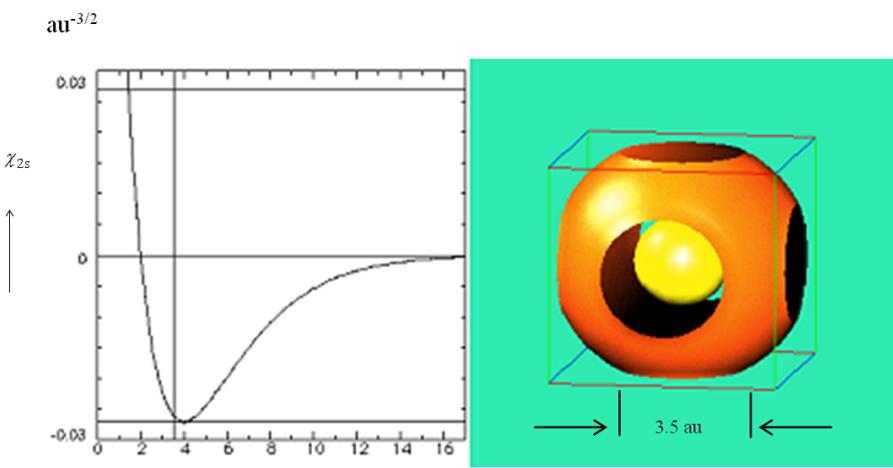


Figure 2. Concentric spheres representing the isosurfaces of the  $\chi_{2s}$  atomic orbital ( $a = \pm 0.027 \text{ au}^{-3/2}$ ) [3].

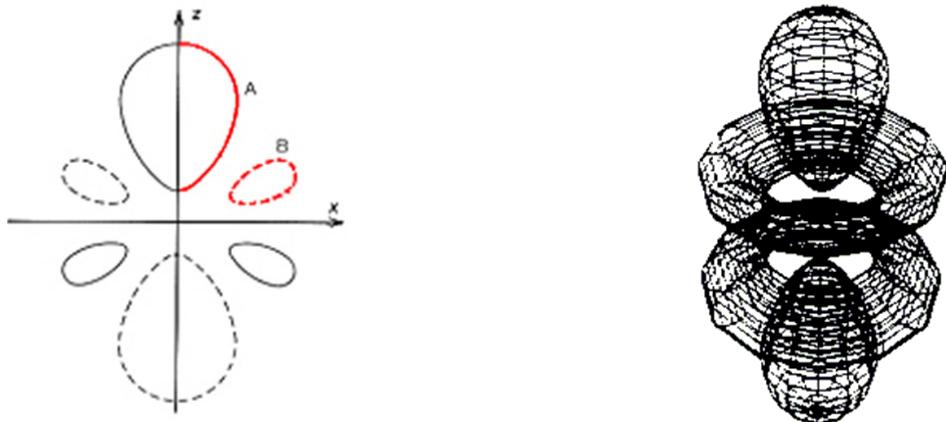


Figure 3. Contour map of hydrogen  $4f_{5z^3-3zr^2}$  atomic orbital which has the function values of  $+0.005$  (solid line), and  $-0.005 \text{ au}^{-3/2}$  (broken line) [17].

Figure 4. Wireframe representation of hydrogen  $4f_{5z^3-3zr^2}$  atomic orbital

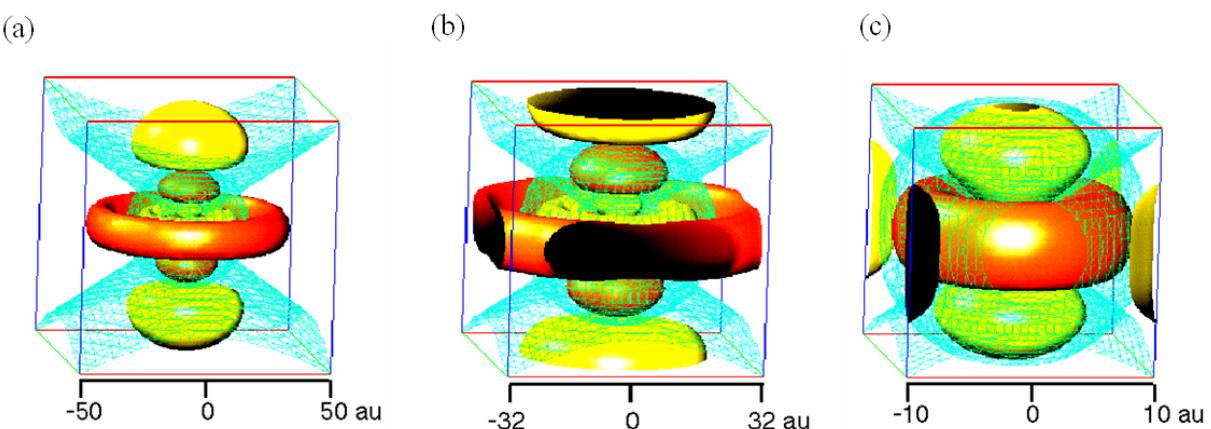


Figure 5. Schematic representation [4] of hydrogen  $\chi_{5d_{3z^2-2}}$  atomic orbital: (a) in the cube of  $100 \times 100 \times 100$ ; (b) in the cube of  $64 \times 64 \times 64$ ; (c) in the cube of  $20 \times 20 \times 20 \text{ au}^3$

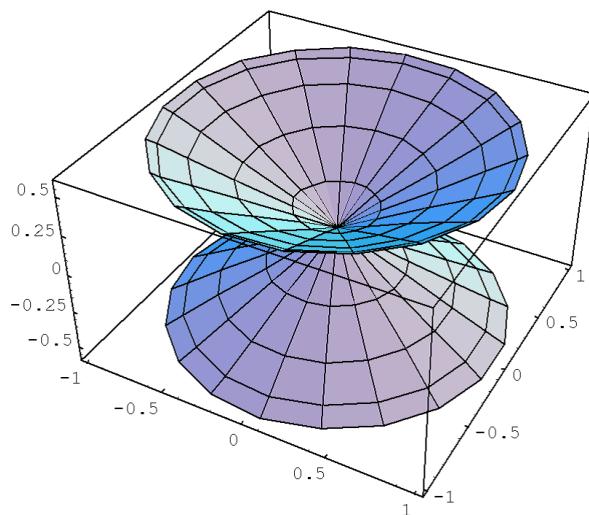


Figure 6. Two conical nodes of  $\theta = 54.7^\circ$  (the upper part) and  $\theta = 125.3^\circ$  (the lower part)

When the absolute value of the magnetic quantum number equals or is larger than 1, the hydrogen atomic orbital has an antisymmetric axis  $C_{|m|}z$ . The hydrogen atomic orbital having an even value of  $l + |m|$  is symmetric and an odd value of  $l + |m|$  is antisymmetric with respect to  $\sigma(xy)$ .

The total number of the nodal surface of hydrogen atomic orbital is  $n-1$ . The  $\chi_{1s}$  orbital has no nodal surfaces. When the azimuthal quantum number equals to 0, namely, 1s, 2s, ..., the orbital has  $n-1$  spherical nodes. When the azimuthal quantum number equals 1, the atomic orbital has a single planar node and  $n-2$  spherical node(s).

When the azimuthal quantum number  $l$  is larger than 1 and the magnetic quantum number  $m$  equals 0, the atomic orbital has two conical nodes and  $n-3$  spherical nodes ( $l$ : even) or  $n-4$  spherical node and a single planar nodes ( $l$ : odd). For example,  $\chi_{5d_{3z^2-r^2}}$  orbital ( $n=5, l=2, m=0$ ) has two conical nodes of  $\theta = 54.7^\circ$  and  $\theta = 125.3^\circ$  (Figure 5 and Figure 6) and two spherical nodes (Figure 5 (b) and (c)).

When the absolute value of the magnetic quantum number  $m$  is larger than 0, the atomic orbital has  $|m|+1$  planar node(s) including Z axis and 0 ( $l$ : odd) or 1 ( $l$ : even) planar nodes of XY plane, and  $n-|m|-2$  ( $l$ : odd) or  $n-|m|-3$  ( $l$ : even) spherical node(s).

The above discussion about the symmetry operation and the information about the shape and number of nodes facilitates to minimize the drawing duration to obtain isosurfaces. Several symmetry operations are already included in our recent software. The software [18] will be distributed on request.

### 3 Conclusion

Consideration of symmetry elements in hydrogen atomic orbitals was shown to facilitate efficient drawing of their isosurfaces.

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