VISUALIZATION OF FOUR DIMENSIONAL ATOMIC ORBITALS

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Four dimensional hydrogen atomic orbital was investigated by a projection method to three dimensional space. The actual outputs were drawn on a two dimensional plane. Transparent plastic block mixed with a certain photochromic compound is expected to support the above visualization.

Keywords: Atomic orbital; Visualization; Four dimension; Projection

INTRODUCTION

Calculations based on quantum mechanics, for example, molecular orbital methods are becoming useful to design organic materials including photochromic compounds [1-2]. Visualizing atomic orbital is important to image the character of an electron which has a duality of a particle and a wave. Four dimensional atomic orbitals [3] are expected to be useful for better and more general understanding of three dimensional orbitals. This paper deals with the visualization of angular part of four dimensional atomic orbitals by the projection method.

RESULTS AND DISCUSSION

Angular Part of Hydrogen Atomic Orbitals

In hydrogen atomic orbital, two to four dimensional angular parts of s orbital and p_y orbital are expressed as equation (1) – (15), respectively [3–6], where their normalization factors have been removed.

Angular part equations on two dimensional *x*, *y* plane:

$$x = r \sin\theta \quad (1)$$

$$y = r \cos\theta \quad (2)$$

s orbital: $Y(\theta) = 1, \quad r^2 = x^2 + y^2 \quad (3)$

p_y orbital: $Y(\theta) r = y, \quad r^2 = x^2 + y^2 \quad (4)$

Angular part equations on three dimensional *x*, *y*, *z* space:

$$x = r \sin\theta \cos\varphi \quad (5)$$

$$y = r \cos\theta \sin\varphi \quad (6)$$

$$z = r \cos\theta \quad (7)$$

s orbital: $Y(\theta, \varphi) = 1, \quad r^2 = x^2 + y^2 + z^2 \quad (8)$

p_y orbital: $Y(\theta, \varphi) r = y, \quad r^2 = x^2 + y^2 + z^2 \quad (9)$

Angular part equations on four dimensional *x*, *y*, *z*, *w* space:

$$x = r \sin\theta \cos\varphi \quad (10)$$

$$y = r \sin\theta \sin\varphi \cos\rho \quad (11)$$

$$z = r \sin\theta \sin\varphi \sin\rho \quad (12)$$

$$w = r \cos\theta \quad (13)$$

s orbital: $Y(\theta, \varphi, \rho) = 1, \quad r^2 = x^2 + y^2 + z^2 + w^2 \quad (14)$

p_y orbital: $Y(\theta, \varphi, \rho) r = y, \quad r^2 = x^2 + y^2 + z^2 + w^2 \quad (15)$

Two to four dimensional s orbital

The equation (3) of an s orbital on two dimensional *x*, *y* plane stands for a circle (Fig. 1 (a)). The equation (8) of an s orbital on three dimensional *x*, *y*, *z* space stands for a sphere [7]. When *z* value in equation (8) is fixed to 0, 4, 8, and 12, we obtain circles A, B, C, and D (Fig. 1 (b)). Projections of these circles on *x*, *y* plane give concentric circles, each of which corresponds to two dimensional

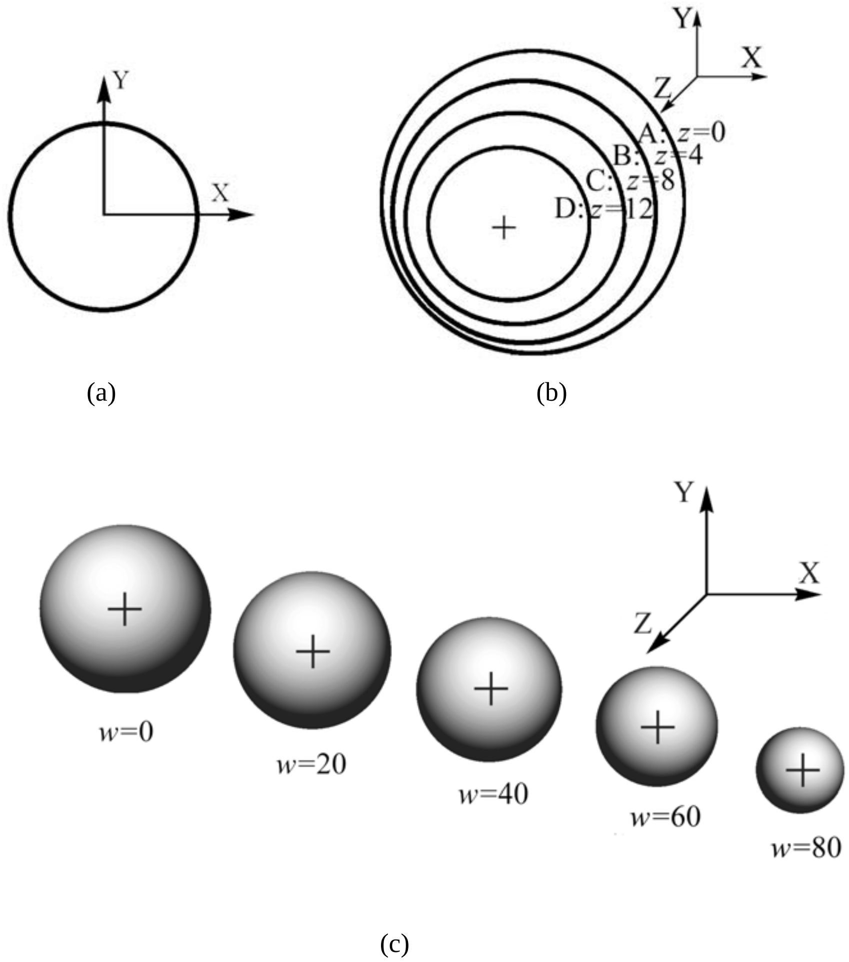

FIGURE 1 Angular parts of s orbitals: (a) visualization of a two dimensional s orbital (3); (b) cross sections (A, B, C, and D) of a three dimensional s orbital (8) on x, y plane (z = 0, 4, 8, and 12, $r^2 = x^2 + y^2 + z^2$); (c) projections of a four dimensional s orbital (14) on three dimensional x, y, z space (w = 0, 20, 40, 60, and 80, $r^2 = x^2 + y^2 + z^2 + w^2$).

circle in Fig. 1 (a). Plus sign in Fig. 1 (b) expresses the sign of the function value. As the z value becomes large, the size of the circle becomes small. A combination of these circles in Fig. 1 (b) gives the original spherical shape of three dimensional s orbital (8).

Equation (14) expresses a four dimensional sphere on four dimensional x, y, z, w, space. When w value in equation (14) is fixed to 0, 20, 40, 60, and 80, we obtain spheres (Fig. 2 (c)) as projections of four dimensional spheres on three dimensional x, y, z space. As y value becomes large, the size of the sphere becomes small in analogy with the size of the circles in Fig. 1 (b). We obtain the shape of four dimensional s orbital by the accumulation of these projections on three dimensional x, y, z space.

Two to four dimensional p orbital

The equation (4) of a two dimensional p_y orbital stands for two circles centred on y axis (Fig. 2 (a)). One of the circles has a value of plus, and the other has a value of minus. The equation (9) of a three dimensional p_y orbital stands for two spheres centred on y axis (Fig. 2 (b)) [7-12]. One of the spheres has a value of plus, and the other has a value of minus. When z value in equation (9) is fixed to 0, 6, 12, 18 and 24, we obtain two circles as cross sections of a three dimensional p_y orbital (Fig. 2 (b)). As the z value becomes large, the size of the circles becomes small, and the interval between the circles becomes large.

When w value in equation (15) of a four dimensional p_y orbitals is fixed to 0, 10, 20, 30, and 40, we obtain a set of spheres (Fig. 2(c)) as three dimensional projection on x, y, z space. One of the spheres has a value of plus, and the other has a value of minus. As the w value becomes large, the size of the spheres becomes small, and the interval between the circles becomes large, in analogy with the relationship of size and distance in Fig. 3 (b). These set of spheres will give the original shape of four dimensional p_y orbital.

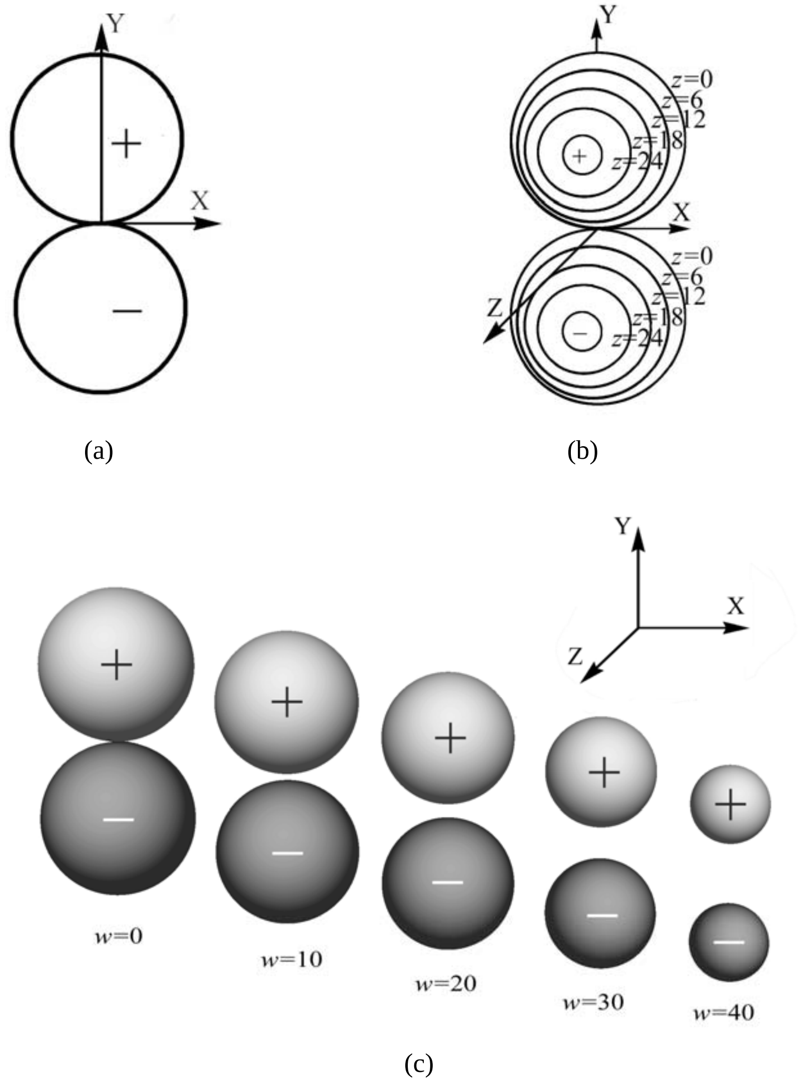

FIGURE 2 Angular parts of p_y orbitals: (a) visualization of a two dimensional p_y orbital (4) on two dimensional *x*, *y* plane; (b) cross sections of a three dimensional p_y orbital (9) (z = 0, 6, 12, 18 and 24, $r^2 = x^2 + y^2 + z^2$); (c) projections of a four dimensional p_y orbital (15) on three dimensional *x*, *y*, *z* space (w = 0, 10, 20, 30, and 40, $r^2 = x^2 + y^2 + w^2 + z^2$).

CONCLUSION

Through a systematic visualization method based on the visualization of an (n-1)-dimensional projection of n-dimensional angular parts, several topological analogies were found. The original shape of n-dimensional angular parts has obtained by the set of an (n-1)-dimensional projection. All figures presented on this paper are drawn on a two dimensional plane. Transparent plastic block mixed with a certain phtochromic compound is expected to visualize these figures in a three dimensional space.

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