The electronic structure of atoms in *N*-dimensional space

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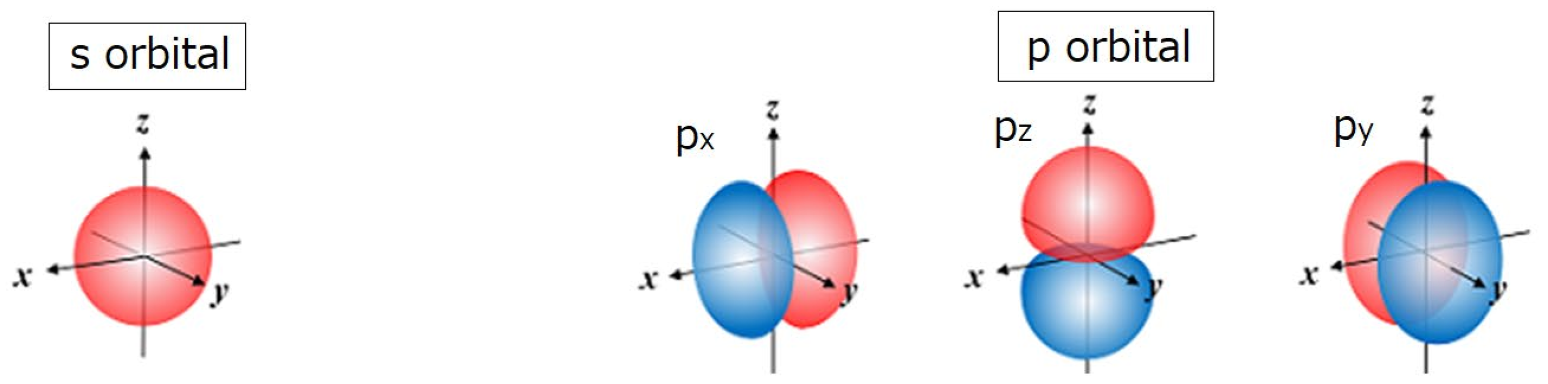
Motivation

It is known that the structure of the electrons that make up the atom is obtained by solving the three-dimensional Schrödinger equation $H\psi = E\psi$.

→ How are the electrons of atoms arranged in 2D or 4D space?

The electronic structure of atoms

The electronic structure of atoms in 3D space.



n	1	2	3	4	5	6
2-Zn	2	8	18	32	50	72

Let D-Z_n be the maximum number of electrons present in the nth electron shell in D-dimensional space. In the case $D = 3$, we have 3-$Z_n = 2n^2$

→ What is the number of 2-Z_n in 2D space for any n?

What is the number of 4-Z_n in 4D space for any n?

Study of 2 dimensional Schrödinger equation

Schrödinger equation

$$\Delta u+\frac{2m}{\hbar}(E-V)u=0$$

Polar transformation →

$x = r\sin\varphi,\ y=r\cos\varphi,\ V = -\frac{e^2}{r}$

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial}{\partial\theta}\right]u+\frac{2m}{\hbar}\left(E+\frac{e^2}{r}\right)u=0$$

→

1. Obtain two equations by separation of variables
2. Solve the equations
3. Find the number of 2-Z_n in 2D space for any n.

1. Obtain two equations by separation of variables

Let $u(r,\theta) = R(r)\Theta(\theta)$. Then we obtain follows.

$$\frac{d^2\Theta}{d\theta^2}+\lambda\Theta = 0 \quad \cdots (1)$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left[\frac{2m}{\hbar}\left(E+\frac{e^2}{r}\right)-\frac{\lambda}{r^2}\right]R = 0 \quad \cdots (2)$$

where λ is constant.

2.1 Solve the equation (1)

$$\frac{d^2\Theta}{d\theta^2}+\lambda\Theta = 0$$

boundary conditions:
$\Theta(0) = \Theta(2\pi), \Theta'(0) = \Theta'(2\pi)$ →

$$\Theta(\theta) = (2\pi)^{-\frac{1}{2}}e^{i\mu\theta}$$

$\mu = \pm\sqrt{\lambda}$ and μ is integer.

2.2 Solve the equation (2)

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left[\frac{2m}{\hbar}\left(E+\frac{e^2}{r}\right)-\frac{\lambda}{r^2}\right]R = 0$$

$\varepsilon^2 := -\frac{2m}{\hbar^2}E,\quad \varepsilon n := \frac{me^2}{\hbar^2}$ ↓ $x := 2\varepsilon r,\quad S(x) := R(r)$

$$S''+\frac{1}{x}S'+\left[\frac{n}{x}-\frac{1}{4}-\frac{\mu^2}{x^2}\right]S = 0$$

$L(x) := x^{-\mu}e^{x}S(x)$ ↓

$$xL''+(2\mu+1-x)L'+\left(n-\mu-\frac{1}{2}\right)L = 0$$

Thus, $n+\mu-\frac{1}{2}\geq 2\mu \rightarrow n-\frac{1}{2}\geq\mu\geq -n+\frac{1}{2}$ (2n is positive integer)

3. Find the number of 2-Z_μ in 2D space for any μ.

From the condition $n-\frac{1}{2}\geq\mu\geq -n+\frac{1}{2}$, we obtain the following table.

u	1	2	3	4	5	6
N	½	3/2	5/2	7/2	9/2	11/2
2-Zu	2	6	10	14	18	22

Currently, we are studying the 4-dimensional Schrödinger equation for the 4-dimensional virtual hydrogen atom. In this case, we have conjectured that the principal quantum number n of the uth electron shell enveloping the nucleus is equal to $(2u+1)/2$ and 4-$Z_u = u(u+1)(2u+1)/3$.

Table 1. The maximum number D-Z_u of electrons present in the μth electron shell.

	1	2	3	4	5	6	⋯	u	the principal quantum number n
2-Z_u	2	6	10	14	18	22	⋯	$4(2u-1)$	$(2u-1)/2$
3-Z_u	2	8	18	32	50	72	⋯	$2u^2$	u
4-Z_u	2	10	28	60	110	182	⋯	$u(u+1)(2u+1)/3$	$(2u+1)/2$

We can see the same structure as the Pascal Triangle in Table 1.