APPLICATION OF MATHEMATICS CALCULATION FOR MICROSTATES AND DESCRIPTION OF THE p^2 ELECTRON CONFIGURATION

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ABSTRACT
The aim of this research was to compute the number of microstates for p^2 configuration n = 6 and x = 2, for d^2 configuration n = 10 and x = 2 and f^2 configuration n = 14 and x = 2 using Euclidean vectors and the math function factorial as well as to describe in detail the microstates for p^2 configuration n = 6 and x = 2. The following results were obtained: for p^2 configuration n = 6 and x = 2, N = 15 microstates; for d^2 configuration n = 10 and x = 2, N = 45 microstates; for f^2 configuration n = 14 and x = 2, N = 91 microstates. It was established that the 15 microstates of the p^2 configuration. It was found that the 15 microstates of the p^2 electron configuration belonged to three terms as followed: 5 microstates corresponding to the 1D term; 9 microstates to the 3p term and 1 microstate to the 1S term.

Key words: vector, factorial, microstate, p^2 electron configuration

INTRODUCTION
Linear algebra and analytical geometry theory and methods are increasingly applied in chemistry. The states of multi-electron atoms or ions in chemistry are described and classified by two schemes (Russell-Saunders (L-S) and j-j coupling schemes). Both use vectors and factorials.

1. Vectors
Definitions
- A vector is a geometric object that has both magnitude (length) and direction.
- The tail of the vector is the end opposite the arrow. It represents where the vector is moving from.
- The head of the vector is the end with the arrow. It represents where the vector is moving to.
- The zero vector is denoted \( \vec{0} \). It has zero length and all the properties of zero.
- Two vectors are equal if they have both the same magnitude and the same direction.

Two vectors are parallel if they have the same \( (\uparrow\uparrow \text{ or } \downarrow\downarrow) \) or opposite \( (\uparrow\downarrow) \) directions. That is, if the angles of the vectors are the same or 180° different.

Two vectors are perpendicular if the difference of the angles of the vectors is 90° or 270° (1-4).

Magnitude of a Vector
The magnitude of a vector \( \overline{AB} \) is the distance between the initial point \( A(x_1, y_1) \) and the end point \( B(x_2, y_2) \). In symbols the magnitude of \( \overline{AB} \) is written as \( |\overline{AB}| \). If the coordinates of the initial point and the end point of a vector are given, the distance formula can be used to find its magnitude:

\[
|\overline{AB}| = \sqrt{(x_2-x_1)^2 + (y_2-y_1)^2}
\]

(Figure 1).

Let as remark, that \( |\overline{AB}| = |\overline{BA}| \). The directions of the two vectors are opposite, but their magnitudes are the same (1-4).
Direction of a Vector
The direction of a vector is the measure of the angle it makes with a horizontal line. One of the following formulas can be used to find the direction of a vector:

\[ \tan \theta = \frac{y}{x}, \]
where \( x \) is the horizontal change and \( y \) is the vertical change or

\[ \tan \theta = \frac{y_2 - y_1}{x_2 - x_1}, \]
where \((x_1, y_1)\) is the initial point and \((x_2, y_2)\) is the terminal point (1-4).

Operations with Vectors
It is possible to operate with vectors in some of the same ways we operate with numbers. In particular:

Adding and Subtracting Vectors
To add or subtract two vectors, add or subtract the corresponding components.
Let \( \vec{u} = \langle u_1, u_2 \rangle \) and \( \vec{v} = \langle v_1, v_2 \rangle \) be two vectors. Then, the sum of \( \vec{u} \) and \( \vec{v} \) is the vector

\[ \vec{u} + \vec{v} = \langle u_1, u_2 \rangle + \langle v_1, v_2 \rangle = \langle u_1 + v_1, u_2 + v_2 \rangle. \]
The difference of \( \vec{u} \) and \( \vec{v} \) is

\[ \vec{u} - \vec{v} = \vec{u} + ( -\vec{v} ) = \langle u_1 - v_1, u_2 - v_2 \rangle. \]
The sum of two or more vectors is called the resultant. The resultant of two vectors can be found using either the parallelogram method or the triangle method.

Parallelogram Method:
Draw the vectors so that their initial points coincide. Then draw lines to form a complete parallelogram. The diagonal from the initial point to the opposite vertex of the parallelogram is the resultant.

Vector Addition:
1. Place both vectors \( \vec{u} \) and \( \vec{v} \) at the same initial point.
Vector Algebra

\[ \vec{u} + \vec{v} = \vec{v} + \vec{u} \]
\[ (\vec{u} + \vec{v}) + \vec{w} = \vec{u} + (\vec{w} + \vec{v}) \]
\[ \vec{u} + 0 = \vec{u} \]
\[ 1 \cdot \vec{u} = \vec{u} \]

Scalar Multiplication

Scalar multiplication changes the magnitude of a vector, but not the direction. In general,

\[ \vec{u} = \langle u_1, u_2 \rangle \]
\[ k \cdot \vec{u} = \langle k u_1, k u_2 \rangle \]

2. Factorial

In mathematics, the factorial of a non-negative integer \( n \), denoted by \( n! \), is the product of all positive integers less than or equal to \( n \), e.t. \( n! = 1 \cdot 2 \cdot \ldots \cdot (n-2) \cdot (n-1) \cdot n \). In a particular way \( 0! = 1! = 1 \) (1-4).

The aim of this research was to calculate the number of microstates for \( p^2 \) configuration \( n = 6 \) and \( x = 2 \), for \( d^2 \) configuration \( n = 10 \) and \( x = 2 \) and \( f^2 \) configuration \( n = 14 \) and \( x = 2 \) using Euclidean vectors and the math function factorial as well as to describe in detail the microstates for \( p^2 \) configuration \( n = 6 \) and \( x = 2 \).

MATERIAL AND METHODS

It is acknowledged that the movement of an electron in an atom could be represented by the orbital angular momentum. Similarly, the intrinsic motion of the electron is given by the spin angular momentum. Both angular momenta should be presented by vectors which have length and direction. Vectors will be identified by letters, their projections with \( m \) (for a single electron) or \( M \) (for more than 1 electron), and lengths will be represented by \( |m| \) and \( |M| \), respectively. For an electron with quantum numbers \( l \) and \( s \), and orbital and spin angular momenta \( \vec{l} \) and \( \vec{s} \), the total angular momentum describing both motions is a sum of vectors: \( \vec{j} = \vec{l} + \vec{s} \) (5-10).

Both vectors process (rotation of an vector around an axis with only vectors’ initial point lying on the axis; the vector and the axis are under a specific angle). Due to this motion, both vectors described a cone each. The addition of \( \vec{l} \) and \( \vec{s} \) could not be random. The angle between them remains constant in the course of processing. This results from the strict spatial orientation of both vectors. They could be oriented in a way such as their vector sum has strictly defined values of \( j \) projections. Also, the differences between these projections \( (h) \) should be integers (11-19). The above mentioned is illustrated on Figure 6 for an electron on p-AO.

![Figure 6](image-url)

The lengths of vectors are shown below the circles.

**Figure 6.** Addition of vectors of orbital and spin angular momenta for \( |l| = 1 \) and \( |s| = 1/2 \). Both circles represent the space quantization of the total angular momentum \( \vec{j} \). The lengths of vectors are shown below the circles.
Figure 7 depicts the addition of $\vec{L}$ and $\vec{S}$ for 2 electrons on p-AO.

Figure 7. Addition of vectors of orbital angular momentum $\vec{L}$ and spin angular momentum $\vec{S}$ for $|\vec{L}| = 1$ and $|\vec{S}| = 1$.

The total angular momentum $\vec{J}$ or $\vec{J}$ for one or more electrons, respectively is quantized in space in the same way, as shown on both figures.

**Russell-Saunders coupling scheme. LS scheme**

In the Russell-Saunders scheme, the spin and orbital angular momenta are always summed independently:

$$\vec{L} = \vec{l}_1 + \vec{l}_2 + \ldots + \vec{l}_N = \sum_{i=1}^{N} \vec{l}_i,$$

$$\vec{S} = \vec{s}_1 + \vec{s}_2 + \ldots + \vec{s}_N = \sum_{i=1}^{N} \vec{s}_i.$$

Then the resulting two vectors $\vec{L}$ and $\vec{S}$ are combined to obtain the total angular momentum $\vec{J}$: $\vec{J} = \vec{L} + \vec{S}$.

**j-j coupling scheme**

The combination of angular momenta of a multi-electron atom according to the j-j coupling scheme is done by combining each individual orbital to respective spin momentum $\vec{j}_i = \vec{l}_i + \vec{s}_i$ and thereafter, the total angular momentum is obtained as the sum of individual total angular momenta:

$$\vec{J} = \vec{j}_1 + \vec{j}_2 + \ldots + \vec{j}_N = \sum_{i=1}^{N} \vec{j}_i.$$

This order of combining is derived from the nature of the j-j scheme – each electron determines its own momentum, and then follow the combination of total individual angular momenta of all electrons.

The spin multiplicity is denoted with $2S + 1$. It is added as a superscript to the left of the letter expressing the sum of orbital momenta (electron state). For example, the electron state derived from the electronic configuration $1s^1$ is:

$s = 1/2$ \hspace{0.5cm} $l = 0$ \hspace{0.5cm} $2s+1 = 2$ $^2S$.

The symbol $^2S$ (read as doublet es) is an electron term derived from the electronic configuration $1s^1$ and including two microstates:

$m_s = 1/2$ \hspace{0.5cm} $m_l = 0$;

$m_s = -1/2$ \hspace{0.5cm} $m_l = 0$.

The six microstates of the electronic configuration $2p^1$ are:

$m_s = +1/2$ \hspace{0.5cm} $m_l = 0, -1$;

$m_s = -1/2$ \hspace{0.5cm} $m_l = 0, -1$.

They could be grouped into:

$s = 1/2$ \hspace{0.5cm} $l = 1$ \hspace{0.5cm} $2s+1 = 2$ term. $^2P$.

The symbol $^2P$ (read as doublet pe), and $^2S$ (read as doublet es) are called electron terms. Therefore, electron terms are a group of microstates (or combinations between them) with the same energy.

The Russell Saunders scheme could be illustrated with several examples:

- **Closed shell** — the general rule for this shell type that it always has $S = 0$ and $L = 0$ or term $^1S$.
- **Open shell** — only one of atomic orbitals making up a given electronic configuration without the maximum number of electrons is enough to have an open shell.

The total number of microstates for any configuration can be counted using by following expression (20).

Number of ways of filling electrons N:

$$N = \frac{2(2l+1)!}{x!(2(2l+1)!-x!)} \quad \text{or} \quad \frac{n!}{x!(n!-x!)}$$

$n = 2(2l+1)$ or double of the total number of orbital’s (For s-AO = 2, p-AO = 6, d-AO = 10, f-AO = 14)

$x = \text{Total number of electrons in sub shell.}$

**RESULTS AND DISCUSSION**

So, for $p^2$ configuration $n = 6$ and $x = 2$

$$N = \frac{6!}{2!(6!-2)!}$$

$$N = 15 \text{ Microstates.}$$

For $d^2$ configuration $n = 10$ and $x = 2$

$$N = \frac{10!}{2!(10!-2)!}$$

$$N = 45 \text{ Microstates.}$$
For $f^2$ configuration $n = 14$ and $x = 2$

\[
N = \frac{14!}{2!(14! - 2!)}.
\]

\[
N = \frac{14.13.12.11.10.9.8.7.6.5.4.3.2.1}{12.11.10.9.8.7.6.5.4.3.2.1.2.1},
\]

\[
N = 91.
\]

For instance, for $m_l = 1, m_s = 0, m_{s_2} = 1/2$
and $m_{s_2} = 1/2$, the microstate is \( \left( \frac{1}{1}, \frac{0}{0} \right) \),
whose wave function is $\psi = \hat{\phi}_{m_l} \hat{\phi}_{m_s} \hat{\phi}_{m_{s_2}} = \hat{\phi}_{0}^+ \hat{\phi}_{0}^-$

\[
\begin{array}{c|c|c|c}
M_L & M_S & 1 & 0 & -1 \\
\hline
2 & & \left( \frac{1}{1}, \frac{1}{1} \right) & & \\
1 & & \left( \frac{1}{0}, \frac{1}{0} \right), \left( \frac{1}{0}, \frac{1}{0} \right) & & \left( \frac{1}{0}, \frac{1}{0} \right) \\
0 & & \left( \frac{1}{1}, \frac{1}{1} \right), \left( \frac{1}{0}, \frac{0}{0} \right), \left( \frac{1}{1}, \frac{1}{1} \right) & & \left( \frac{1}{1}, \frac{1}{1} \right) \\
-1 & & \left( \frac{0}{1}, \frac{0}{1} \right), \left( \frac{0}{1}, \frac{0}{1} \right) & & \left( \frac{0}{1}, \frac{0}{1} \right) \\
-2 & & \left( \frac{1}{1}, \frac{1}{1} \right) & & \left( \frac{1}{1}, \frac{1}{1} \right) \\
\end{array}
\]

In Table 1 $M_L$ and $M_S$ denote the projections of respective $L$ and $S$ vectors.
The content of the table becomes clear from Fig. 8 – the numbers 1, 0, -1 are the $m_l$-
projections of the orbital angular momenta of the first and second electron, the signs (+) and (-), placed over $m_l$ indicate the
$m_s$-projections of the spin angular momentum.

**Table 1. Microstates of the electronic configuration $p^2$**

- For $m_l = -1, 0, 1$, and $m_s = 1/2$, the microstate is \( \left( \frac{1}{1}, \frac{0}{0} \right) \),
whose wave function is $\psi = \hat{\phi}_{m_l} \hat{\phi}_{m_s} \hat{\phi}_{m_{s_2}} = \hat{\phi}_{0}^+ \hat{\phi}_{0}^-$

- For instance, for $m_l = 1, m_s = 0, m_{s_2} = 1/2$
and $m_{s_2} = 1/2$, the microstate is \( \left( \frac{1}{1}, \frac{0}{0} \right) \),
whose wave function is $\psi = \hat{\phi}_{m_l} \hat{\phi}_{m_s} \hat{\phi}_{m_{s_2}} = \hat{\phi}_{0}^+ \hat{\phi}_{0}^-$

**Figure 8. Microstates which are derived from the electronic configuration $p^2$.**
A more complex problem arises for wave functions of the second column, where there are two or three microstates within a cell. Let’s take a look on the content of the cell with \( M_L = 1 \) and \( M_S = 0 \).

There are two microstates - \( (1,0) \) and \( (0,1) \).

They could be written as functions
\[
\psi_1 = c_1 (1,0) + c_2 (0,1), \\
\psi_2 = c_3 (1,0) + c_4 (0,1),
\]

the coefficients \( c_1, c_2, c_3, \) and \( c_4 \) are associated with the conditions
\[
c_1^2 + c_2^2 = 1 \\
c_3^2 + c_4^2 = 1
\]

norming
\[
c_1^2 + c_3^2 = 1 \\
c_2^2 + c_4^2 = 1
\]
distribution, reflecting the circumstance that both functions are normed and that every microstate is distributed between both functions in a way such that it is completely depleted.

The system of 4 equations shown above with four variables has a solution
\[
c_1 = c_4 = 1 \\
c_2 = c_3 = 0
\]

and due to the fact that it has \( M_L = 1 \) and projection on the selected axis 1, we obtain a vector with length of \( \sqrt{6} \) and projection on the same axis 2 (in \( h/2\pi \) units).

In other words, the microstate \( (1,1) \) has to be a function of this vector. Once obtained however, this vector is quantized in the space and apart the projection +2, it could be also oriented in a way such as to have projections equal to +1, 0, -1, -2. Also, the orientation of the spins of both electrons should be always opposite. It is important to understand that one of respective combinations in the column with \( M_S = 0 \) belongs to the vector derived from \( (1,1) \). This vector is denoted with the letter D.

The spin multiplicity is \( 2S+1 \), or there is one term \( ^1D \) (singlet de), which includes 5 microstates or combinations, all of which (without exceptions) are arranged vertically in the middle column of Table 1.

As these combinations are unknown to us, we will randomly remove one microstate from each row of the second column as belonging to the term \( ^1D \). The result is illustrated in the new Table 2.

With the new table, we proceed in the same way as with Table 1 – choosing the microstate with highest value for \( M_L \). These are \( (1,0) \), \( (1,0) \), \( (0,1) \). From them, we retain the microstate with maximum value for \( M_S \), i.e. \( (1,0) \). It corresponds to \( M_L = 1 \) and \( M_S = 1 \) or it is derived from vectors \( \vec{L} \) and \( \vec{S} \) each with a length of \( \sqrt{2} \), whose projections could be 1, 0, -1. These two vectors determine the existence of nine microstates with different energy, differing in projections on a random axis. These nine microstates constitute the electron term \( ^3P \). If these microstates (or their combination in the middle column) are removed from Table 2, only one combination of microstates is left, which is not mentioned so far and whose energy in different from the energy of \( ^1D \) and \( ^3P \) terms. It is
\[
3^{-1/2} \left[ \left( \begin{array}{c} 0,0 \\ 1,1 \\ -1,1 \end{array} \right) \right]
\]
and due to the fact that it has \( M_L = 0 \) and \( M_S = 0 \), it forms the term \( ^1S \).
**Table 2. Microstates of p^2 after removing 1D.**

<table>
<thead>
<tr>
<th>M_l</th>
<th>1</th>
<th>0</th>
<th>-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0, 0</td>
<td>1, -1</td>
<td>0, -1</td>
</tr>
<tr>
<td>1</td>
<td>1, 0</td>
<td>0,</td>
<td>0, 0</td>
</tr>
<tr>
<td>2</td>
<td>0, 0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**CONCLUSIONS**

Ultimately, the description of the 15 microstates derived from the electronic configuration p^2 led to the following result. These microstates fell into three energy terms as follows:

- 5 microstates included in the electron term 1D;
- 9 microstates included in the electron term 3P;
- 1 microstates included in the electron term 3S.

**REFERENCES**


