Continuous Groups

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Group theory allows us to study various aspects of chemical compounds and their physical properties. From axis rotation to symmetrical tendencies, it is very useful to a structural chemist. Within the topic of group theory, there are many subtopics, including discreet groups and continuous groups. Molecules are usually associated to discreet groups. Things such as angular momentum and spin are associated to continuous groups. Continuous groups, also called Lie groups, help to tie the chemistry components of group theory and mathematics together even closer. This paper will begin with the basic elements of group theory, then introduce continuous groups, and then give an example of a Lie group.

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I. INTRODUCTION

A group can be defined as a set of objects or operations, rotations or transformations that may be multiplied to form a well-defined product.[1]To be defined as a group, a set of elements must follow certain rules. The four group postulates are:

1. The product of any two elements in the group and the square of each element must be an element of the group.
2. One element in the group must commute with all others and leave them unchanged.
3. There exists an element in each group called the identity. Its multiplicative is equal to 1 and its additive is equal to 0. It may be found in the form of a matrix,

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1}$$

4. The associative law must hold

$$A(BC) = (AB)C. \tag{2}$$

5. Every element must have a reciprocal which is also an element of the group. The reciprocal of a product of 2 or more elements is equal to the product of the reciprocals reversed

$$(AB)^{-1} = B^{-1}A^{-1}.^{2} \tag{3}$$

II. BASIC ELEMENTS OF GROUP THEORY

Groups can also be related to one another. There may exist a function between the two groups. If this correspondence preserves the group multiplication, we say that the two groups are homomorphic, meaning the transformation preserves the operations of the first set. If the correspondence is 1 to 1, still preserving the group multiplication, then the groups are isomorphic, or have the same form.[1] For a crystal, a symmetry group contains a finite number of rotations and reflections. There are two types of groups- discreet and continuous.[1]

III. HISTORY OF CONTINUOUS GROUPS

Credit for introducing continuous groups into literally all branches of math is mainly due to the work of mathematicians Sophus Lie and Felix Klein.[3] Lie is considered to be one of the last great mathematicians of the 19th century, and continuous groups are now more commonly known as Lie groups.[3] Lie and Klein's research was to a certain extent inspired by their deep interest in the theory of groups and in various aspects of the notion of symmetry. However after the initial period of joint studies their areas of scientific work diverged. Lie devoted his life to the theory of continuous groups. His theory rested on his discovery of the intimate connection between continuous groups and specific algebraic systems.[3] Lie concluded that it is always possible to assign a Lie group a corresponding Lie algebra.[3] These groups were used as a tool to solve or simplify ordinary and partial differential equations.[4]

IV. PROPERTIES OF LIE GROUPS

There are two kinds of Lie groups, real Lie groups and complex Lie groups, depending on whether the base manifolds are real or complex manifolds. Both are important and the theories can be constructed in the same way.[5]For purpose here, the focus will remain on real Lie groups. A given Lie group G has a unique universal covering space which can also be defined as a Lie group paired with its respective algebra.[6] A Lie group can also be defined as a topological group which can be equipped with an analytic atlas in such a way that the group operators are analytic. In similar terms, a topological group is said to be a Lie group if it possesses a compatible analytic atlas.[7]

The structure of each group G is described by two basic maps: the multiplication

$$n : G\ x\ G = G, m(ab) = ab \tag{4}$$

and the inverse

$$iG \to Gi(g) = g^{-1}.^{6} \tag{5}$$

If G has an extra geometric structure we require the compatibility o these maps with it. Thus we say that a group G is:

1. a topological group
2. a Lie group
3. a complex analytic group
4. a finite group if F is also:
   - a topological space
   - a differentiable manifold
   - a complex and analytic manifold and
   - if two maps, m, i are compatible with the given structure, ie are continuous, differentiable complex analytic or regular algebraic.[6]

A Lie group can be thought of as an imitation of a topological group. Let G be the topological group. Suppose there is an analytic structure on the set G, compatible with its topology, which converts it into an analytic manifold and for which the map

$$(x, y) \to xy(x, y\ \epsilon\ G)\times \to x^{-1}(x\ \epsilon\ G)\ of\ G \times G \tag{6}$$

into **G** where **G** and **G** are both analytic.[8]

A. Lie algebra

Given a Lie group G, we will associate to it a Lie algebra g (defined as the algebra over a Lie space) and an exponential map

$$exp : g \to G. \tag{7}$$

An algebra with a product [a b] satisfy the antisymmetry axiom and the Jacobi identity is called a Lie algebra. [a, b] is called a Lie bracket.[6]The Lie axiom states that

$$[a, b] = -[b, a] \text{ antisymmetry}^{6} \tag{8}$$

and

$$[a[b, c]] + [b[c, a]] + [c[a, b]] = 0 \text{ Jacobi identity}^{6} \tag{9}$$

Lie algebra, a form of differential geometry, applies to Lie groups. A Lie product states that

$$[a, b] = ab - ba.^{6} \tag{10}$$

The Lie algebra **g** can be defined as the Lie algebra of a vector field acting on **G**. In particular, this applies to linear representations of the Lie algebra. Conversely a homomorphism of Lie algebras integrates to a homomorphism of Lie groups, provided that **G**, is simply connected.[6]The exponential map is obtained by integrating these vector fields proving that, in this case, the associated 1-parameter groups are global. A homomorphism

$$\Phi : G_1 \longrightarrow G_2 \tag{11}$$

of Lie groups induces a homomorphism

$$d\Phi : g_1 \longrightarrow g_2 \tag{12}$$

of the associated Lie algebras.[6]Lie's essential idea was to study elements **R** in a group **G** that are infinitesimally close to the unity of **G**

$$R\Psi = \begin{pmatrix} cos\psi\ sin\psi \\ -sin\psi\ cos\psi \end{pmatrix} = I_2 cos\psi + i\sigma^2 sin\psi = \exp(i\sigma^2\psi).^{1}$$

Rotation of functions and orbital angular momentum in the foregoing discussion the group elements are matrices that rotate the coordinate ds. Now let us hold the coordinates fixed and rotate a function

$$\Psi(xyz) \tag{13}$$

relative to our fixed coordinates **x' = R(x)**

$$R\Psi(xyz) = \Psi'(xyz) = \psi x'.^{1} \tag{14}$$

V. USES OF LIE GROUPS

The electron at rest can exist in two independent states, which can be labeled as "spin up" and "spin down." To describe a particle with two internal degrees of freedom, we must set up a two-component wave function to represent the particle[9]

The electron will translate from an SU(2, c) group to an SO(3, r) group, since SO(3, r) is a 2 $\rightarrow$ 1 homomorphic image of SU(2, c). By definition, SO (3, r) is a three-dimensional special orthogonal rotational group, where SU(2, c) is a 2x2 matrix defined as a special unitary group.[9]

Consider the U_2 group of 2 x 2 matrices. Any Hermitian 2x2 matrix may be written as a linear combination of the following four matrices:[10]

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{15}$$

$$\tau_\mathrm{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{16}$$

$$\tau_\mathrm{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{17}$$

$$\tau_\mathrm{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{18}$$

letting these four matrices being defined as he infinitesimal operators of the group U_2. If the unitary matrices are restricted to having a determinate equal to +1, then the group is called SU_2. The restriction from U_2 to SU_2 simply removes the freedom to change the phase of both states of the single nucleon simultaneously. These matrices are the same as the spin matrices for a particle with s = 1/2.[10]

We will use this to show the SU(2)→ SO(3) 2→1 homomorphism. The 2→1 ratio can be interpreted that as for every two items of SU(2), there is 1 item in the SO(3) matrix.[9]

$$\psi = u_1(x)\begin{pmatrix}1\\0\end{pmatrix} + u_2(x)\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}u_1(x)\\u_2(x)\end{pmatrix}. \tag{19}$$

The state space describing such a particle is then a tensor product space of the form

$$C_2 \bigotimes H_4. \tag{20}$$

The C_2 is a complex two-dimensional space, called a spinor space, and H_4 is a Hilbert space of complex-valued functions defined on four-dimensional space-time.[9]

Figure one shows the visualization of the two independent internal states of the electron. If we rotate the vector $|v>$ in C_2 four successive times through $\Pi/2$ we return to our starting place. However, our physical picture for the spin has rotated through 4Π.[9]

Figure 2 shows these operations. The states

$$\pm|v_{\frac{1}{2}}> \tag{21}$$

both represent an electron in the spin up state, whereas

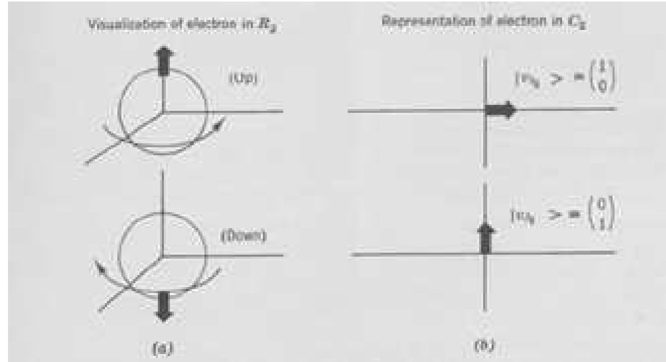

FIG. 1: When the electron is in a "spin up" state (top right), we represent it in a complex two-dimensional space C_2 (top left). The "spin down" state is represented by bottom right and bottom left respectively.

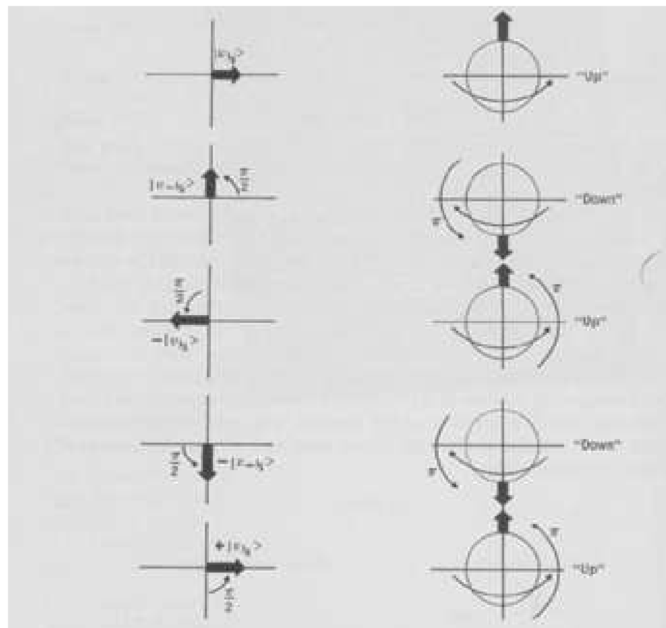

FIG. 2: As we rotate a state $|v>$ in a C_2 successfully four times through $\pi/2$ about any fixed axis, we wind up where we started. In the meantime, the representative of the physical state in R3 has returned twice to its original orientation. We have transferred the Homomorphism that exists between the groups SU(2,c) and SO(3, r) onto the vector spaces C_2 and R_3 in which these groups act as changes of bases.

$$\pm|v_{\frac{-1}{2}}> \tag{22}$$

both represent an electron in the spin down state.[9]

This is a manifestation of the 2→1 nature of the group homomorphism SU(2,c)→ SO(3,r) in terms of the vector spaces on which these groups act.

A2Π rotation of the axes in R_3, which leaves R_3 unchanged, should have no effect on the measurement of the electron spin, even though it corresponds to a Π rotation in C_2. This is true, since only the matrix elements of the spin are measurable:[9]

$$< \phi|\sigma|\phi > \tag{23}$$

Under a Π rotation in C_2, the matrix elements become

$$< \phi|e^i\theta \cdot \sigma/2\dagger\sigma e^i\theta \cdot \sigma/2|\psi > \equiv < \phi|-I_2\sigma-I_2|\psi > = < \phi|\sigma|\psi > \tag{24}$$

It is exactly this quadratic transformation property of matrix elements which allows us to associate two unitary operations of SU(2) with each physical rotation operation of SO(3).[9]

VI. CONCLUSION

In the end, it is evident that not only is group theory important and terribly useful, but the Lie (continuous) groups, with their particular rules, largely bridge the gaps between chemistry, physics, and mathematics. By writing the spin example in terms of a Lie group and algebra, we can see their importance in the field of quantum mechanics.

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