INTERNATIONAL JOUNAL OF: SCIENCE RESEARCH AND TECHNOLOGY

TIMBOU-AFRICA ACADEMIC PUBLICATIONS
INTERNATIONAL JOURNAL, MAY, 2022 EDITIONS
VOL. 9 NO. 9 ISSN: 2623-7861

APPLICATION OF LIE ALGEBRA TO 3-D HYDROGENIC ATOM

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ABSTRACT

Lie algebraic method to simple quantum system was examined. Lie algebra were discussed generally with properties and types. The calculus commutators were also analyzed. The realization of SO (2,1) lie algebra was discussed and it was applied to 3-dimensional hydrogen atom.

Keywords: Lie, algebra, hydrogen, quantum, atom.

INTRODUCTION

Algebraic techniques based on dynamical groups have been successful and useful in the description of bound states and resonances in Nuclear and Atomic physics (Wybourne, 1974). These techniques have proved useful tools in the analysis of bound states problems, ranging from exact solutions, as the coulomb by Engel field (1972) and harmonic oscillator potentials by Moshinsky (1968), to algebraic models of physical systems, such as the InteractingBosonMod5 (IBM) description of collective states in nuclei (Arima and lachello, 1976, 1977 and 1979). IBM has been especially useful in the understanding of nuclear spectra and electromagnetic transitions (Isacker et.al., 1997; Levai et.al, 1998; Garcia-Ramos and I sacker, 1999). Aphasic et.al. 1983 have shown that bound and scattering states of certain one-dimensional potentials can be related to unitary representation of a certain group and its analytic continuation to a non-compact group respectively. Frank and Wolf, 1984 considered the bound and scattering states for the potential by using a new Lie-algebraic framework. The simplex relationship between the energy eigen states of a d-dimensional hydrogen atom and those of a D-dimensional harmonic oscillator in terms of the

SU(1, 1) algebra have been discussed by Gao-Jian et al. (1994).

In a recent series of papers (Dong 2003, 2004; Dong et. Al 2004, 2005), have applied dynamical group approach to variety of simple quantum systems in terms of the SU(1, 1) dynamical algebra, by constructing the ladder operators (creation and annihilation operators) for some given wave functions and then constitute a suitable dynamical group.

Methodology

Dynamical groups used were special linear group SL (m, c), Symplectic group Sp (k, c), and general linear Lie algebra.

Lie algebra involves the use of the basic concept of vector spaces, linear transformation and operators, matrices and commutators. A linear algebra is defined over a field F(real or complex) as a vector space a over F having a bilinear law of composition which is denoted by A o B with the following properties:

(i) A o B ϵ σ
(ii) A o (B+C) = A o B + A o C
(iii) (A+B) o C = A o C + B o C
(iv) α (A o B) = (α A) o B = A o (α B)

for all α ϵ F and A, B, C ϵ σ

The first property satisfies the closure property while (ii) and (iii) are right and left distributive over the addition. The scalar property α is distributive over the multiplication of A and B. Combining the above properties we have the bilinearity rule:

$$\left(\sum_j \alpha_j A_j\right) o \left(\sum \beta_k \beta_k\right) = \sum_{jok} \alpha_j \beta_k (A_j \; o \; B_k)$$

where $\alpha_j \beta_k \quad \in \; F \; and \; A_j, B_k \; \in \sigma$

A Lie algebra L is a vector space with a particular binary operation defined on it i.e. Lie algebra is a vector space with a binary operation (x, y) ϵ L x L………… [x, y] ϵ L which is called Lie bracket or commutator which satisfies the following properties;

(i) [x, y] ϵ L
(ii) [x, y + z] = [x, y] + [x, z]
(iii) α [x, y] — [αx, y] = [x, αy]
(iv) [x, y] = - [y, x]

(v) [x,[y, z]] + [y,[z, x]] + [z,[x, y] = o
For all α ϵ F and x, y, z ϵ L.
Observing the properties above, it is observed that Lie algebra is a law of linear algebra with the additional rules (iv) and (v). Rule (iv) shows that Lie multiplication is not associative, it is called Jacobi identity and replaces rule x o (y o z) = (x o y) o z of an associative algebra. Rules (ii) and (iii) retains the fundamental bilinearity rule. A Lie algebra is real or complex when vector space is respectively real (F = R) or complex (F = C). Some Lie algebras differ only in the names of elements, everything else being the same such Lie algebras are Isomorphic.
A subset K of a Lie algebra is called a sub-algebra of L if for x, y ϵ K and α, β ϵ F the following holds;
(i) $\alpha x + \beta y \in K,$
(ii) $[x, y] \in K$
From the two conditions above, it is obvious that a sub-algebra K of a Lie algebra is also a Lie algebra. A special type of sub-algebra is called an ideal of a Lie algebra L with the property $[I, L] \in I$, it implies for all $x \in I$ and $y \in L$, $[x, y] \in I$ holds. Every Lie algebra has at least two ideals namely the Lie algebra itself and the sub-algebra O consisting of the zero elements only i.e. $0 = \{O\}$.
A Lie algebra is said to be solvable if $L_n = 0 \; for \; some \; n \in N$.
A Lie algebra is said to be nilpotent if $L^n = 0 \; for \; some \; n \in N$.
A Lie algebra is said to be abelian if $[x, y] = 0 \; for \; all \; x, y \in L$.
Generally, Lie algebra is neither associative nor commutative but it can often be obtained from an associative algebra σ of matrices, linear transformation or linear operators on some vector space. This can only be done by defining the Lie multiplication of two elements $A, B \in \sigma$ as the commutator $[A, B] = AB - BA$.
The special Linear group SL(n, c), the Orthogonal group O(n, c), the Symplectic group SP(n, c) and Special Orthogonal group SO(n, c) are called dynamical groups. They are subgroups of the General Linear group GL(n, c).
A realization of a Lie algebra is a homomorphism which associates a concrete set of operators with each abstract basis vector of the Lie algebra. It is more of physical concept than a Mathematical concept and it is of great importance in the application of Lie algebra.
In Quantum mechanics such operators are often differential operators expressed in terms of the position and momentum operators q and p. However, the realization may also be expressed in terms of matrix operators. There are two

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ISSN: 2623-7861

ways to approach this connection between operators and abstract basis vectors. One approach is to begin with an abstract Lie algebra and to find a suitable set of operators which satisfy the same commutation relations as the abstract basis of the Lie algebra. Another approach is to reverse the first method by finding physically combined operators and evaluate its commutation relation. If such an operator exist and satisfy closure property then, it is a realization. Then, their union is a basis of larger Lie algebra if the commutators of the form $[A_j, B_k]$ can be expressed as linear combination of the operators in $A \cup B$. Otherwise, we must extend $A \cup B$ to include the set $C^{(1)}$ of operators $C_i^{(1)}= [A_s, B_k]$which are not expressed in this form.

Considering the three component $L_j,\ j = 1, 2, 3$ of the orbital angular momentum $L = r\ x\ p$, where $r = (x_1, x_2, x_3)$ is the position vector in $R\ and$ $P = -i\,\nabla$ is the momentum vector. The realization of the basis vectors of the Lie algebra SO(3) can be provided since they satisfy the commutation relations;

$[L_1, L_2] = iL_3, [L_2, L_3] = iL_1, [L_3, L_1] = iL_2$

which can be written together as;

$$[L_j, L_k] = i \sum C_{jkl} L_i.$$

Another set of commutation relations can be obtained using the lader operators which can also be called raising and lowering operators.

$L+= L_1 + iL_2$

$L-= L_1 - iL_2$

Then the commutation relations among $L_+, L_-\ and\ L_3$ are given by;

$[L_+, L_-] = 2L_3$

$[L_3, L_+] = L_+$

$[L_3, L_-] = -L_-$

Result and discussion

The Hamiltonian for the 3-dimensional hydrogen atom in atomic units ($m = e = h = l$)is

$$H = \frac{1}{2}P^2 - \frac{Z}{r} - (1)$$

where Z is the nuclear charge. Substituting for P in (1)

$$H = \frac{1}{2}P_r^2 + \frac{L^2}{2r^2} - \frac{Z}{r} - (2)$$

and the schrodinger equation for the energy E is

$$(H — E)\Psi(r) = 0 ------------------- (3)$$

The Hamiltonian is not directly expressible in terms of the SO (2, 1) generators. However, if (3) is multiplied on the left by r and scaling transformation is introduced from the physical operators {r, P_r} to the model space operators $\{R, P_R\}$given by

$$r = \gamma R, P_r = \frac{1}{\gamma} P_R -----------------(4)$$

then (3) can be expressed as

$$\left(\frac{1}{2}\gamma r P_r^2 \ + \frac{L^2}{2r} - Z - \ Er\right)\Psi(r) = 0$$

$$\left(\frac{1}{2}\gamma r P_r^2 \ + \frac{\gamma L^2}{2r} - \gamma Z - \gamma Er\right)\Psi(r) = 0 \text{----------------------------}(*)$$

From (4): $R \ = \frac{r}{\gamma} \ = \ P_R \ = \gamma P_r$

(*) becomes;

$$\left[\frac{1}{2}\left(PR_R^2 + \frac{L^2}{R} \ 2\gamma^2 ER\right) - \gamma Z\right]\psi(\gamma R) = 0$$

If we use model space operator and choose $a = 1$ in the realization of T_1, T_2 and T_3 to obtain

$$T_1 = \frac{1}{2}\left[RP_R^2 \ + \frac{\tau}{R} - R\right] -------------- (5)$$

$$T_2 \ = \ RP_R \ ------------------ (6)$$

$$T3 \ = \frac{1}{2}\left[RP_R^2 \ + \frac{\tau}{R} + \ R\right] ------------ (7)$$

If $\gamma \ and \ \tau$ is chosen such that

$$2\gamma^2 E \ = \ -1 ------------------ (8)$$

$$\tau \ = L^2 ------------------(9)$$

then $a \ T_3$ eigenvalue equation is obtained:

$$(T_3 \ - \gamma z)\psi \ (\gamma R) = \ 0 ------------- (10)$$

Since the hydrogen atom wave function $\psi(r)$ are separable in spherical coordinates.

$$\psi(r, \theta, \phi) = \phi(r) rim \ (\theta,) ------------- (11)$$

as products of a radial function and a spherical harmonic it follows that (3) or (10) can be reduced to eigenvalue equation for the radial function if we replace L^2 by its eigenvalue l(l + 1). Therefore

$$(H — \ E)\theta(r) = \ 0 ------------------(12)$$

TIJSRAT
ISSN: 2623-7861

$$(T_3 \ - \gamma z)\phi(R) = \ 0 ----------------- \ (13)$$

where $\phi(R) = \phi(\gamma R) ----------------------- (14)$

It follows from *(35)* $(since \ a \ = \ 1, \tau \ = \ L^2)$ that

$$K \ = \frac{1}{2}[-1 \pm (2l + 1)]$$

Since $1 \ \ \geq 0 \ and \ K \ > \ -1$, positive sign must be chosen to obtain

$$K \ = \ l ------------------- \ (15)$$

$$q \ = \ l \ + \ 1 \ + \ \mu, \mu = \ 0, 1, 2 \ldots ------(16)$$

where q is an eigenvalue of T_3 and from 45 and (47) the scaling factor and energy are

$$\gamma = \frac{q}{z} -------------------- (17)$$

$$E \ = Eq = -\frac{z^2}{2q^2} \ \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (18)$$

This is the famous Bohr formula for the energy levels of the hydrogen atom if a is identified with the principal quantum number n.

There are several important ideas related to the above derivations. The choice $2\gamma^2 E \ = \ 1$ instead of *(8)* would lead to positive energies corresponding to scattering states and a T_1 eigenvalue equation. Our interest lies in bound states so (13) justifies our earlier choice of $\{T^2, T_3\}$ as the set of commuting operators to diagonalize. It is also important to realize that (5) to (7), with the specific choice (9) of τ, do form a realization of SO(2, 1). This follows since the component of l_j of the orbital angular momentum (and hence L^2) commute with the SO(2, 1) generators.

$$[L_j, T_k] = \ 0, j, k \ = \ 1, 2, 3 -------------- (19)$$

This follows that the T_3 eigen functions can be labeled as

$$\psi_{nlm}(R, \theta, \phi) = \phi_{nl}(R)\gamma_{im}(\theta, \phi) ----------- (20)$$

The most important aspect of the derivation of (13) from (12) is that the scaling transformation and pre-multiplication of the schrodinger equation by τ is a non-unitary transformation. This is clear since the discrete state spectrum of H is not complete for bound state wave functions (the continum states also contribute) whereas the spectrum of T_3 is purely discrete and complete. Thus, the eigen functions of (10) and (13) are not the usual hydrogenic ones so we call them the scaled hydrogenic Eigen functions. Moreover, the SO(2, 1) generators given by the realization T_1 , T_2 and T_3 are not hermitian with respect to the usual scalar product and the T3 eigen function do not form an orthonormal set with respect to

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ISSN: 2623-7861

it. This is not a disadvantage since it could be shown that a new scalar product can be chosen with respect to which the T_k are hermitian.

Conclusion

This research work has successfully analyzed the Lie algebraic method and this is use to solve simple quantum system. The quantum system considered is 3-dimensional hydrogenic atom using SO (2, I) Lie algebraic method. Lie algebra as a whole was introduced with the analysis of its properties. After which its properties were compared with properties of linear algebra and their differences were analyzed. Lie algebra is an interesting approach to many physical systems such as quantum systems. It can also be used in special relativity. Lie algebraic method may not be appreciated till it is practically applicable to desired system.

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TIJSRAT
ISSN: 2623-7861