# Theorems on the Jordan-Schwinger Representations of Lie Groups and its Application to the Algebraic Hamiltonian for Vibron Model of Diatomic Molecules

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The most general algebraic Hamiltonian for vibron model of diatomic molecules is obtained by using the theorems on the Jordan Schwinger representations of Lie groups.

## Introduction

We shall first discuss a general transformation thoery of the boson creation and annihilation operators under a Jordan-Schwinger representation[1] of a Lie group. As an application of the theory we shall construct the most general algebraic Hamiltonian for a diatomic molecule based on the U(4) vibron model.[2,3] This will be achieved by classifying the boson operators into scalars and vectors under orthogonal transformation instead of using the ordinary irreducible tensor method.[2] It is an extension of the previous work[3] where we have constructed an Hamiltonian which contains terms up to the fourth order in the generators of U(4) and describes the interaction between the rotational and vibrational degrees of freedom.

## The Theorems on the Jordan-Schwinger Representations

Let $L^{(s)}$ be a Lie group of $s$-dimensional matrices and $T = ||t_{ik}||$ be a generator. Then the Jordan-Schwinger representation of $T$ is defined by

$$T = a^+ \cdot T \cdot a = \Sigma t_{ik} a_i^+ a_k, \tag{1}$$

where $a^+ = (a^+_1, a^+_2, \bullet\bullet\bullet, a^+_s)$ and $a = (a_1, a_2, \bullet\bullet\bullet, a_s)$ are sets of boson creation and annihilation operators in a $s$-dimensional boson field satisfying the commutation relations

$$[a_i, a_k^+] = \delta_{ik}, \quad [a_i, a_k] = [a_i^+, a_k^+] = 0. \tag{2}$$

Since $a^+_i$ is the hermitian adjoint of $a_i$, the Jordan-Schwinger representation $T$ satisfies the symmetry property,

$$(T)^+ = (T^+) = a^+ \cdot T^+ \cdot a. \tag{3}$$

The Jordan-Schwinger-representation provides a faithful representation of the Lie algebra corresponding to $L^{(s)}$.

Hereafter we shall limit the discussion to a Lie group $L^{(s)}$, where any element $U$ of the group can be expressed in terms of an appropriate generator $T$ in the exponential form

$$U = \exp(T) \in L(s) \tag{4}$$

Then the Jordan-Schwinger operator $\check{U}$ corresponding to $U$ is defined by

$$\check{U} = \exp(\hat{T}), \tag{5}$$

which satisfies the symmetry properties

$$(\check{U})^+ = (U^+)^v, \ (\check{U})^{-1} = (U^{-1})^v \tag{6}$$

where + denotes the hermitian adjoint and $v$ denotes the Jordan-Schwinger operator.

The Jordan-Schwinger operator $\check{U}$ has the following properties:

1) The transformation of the creation and annihilation operators $(a^+_i, a_k)$ under $\check{U}$ are described by the original matrix $U$ as follows

$$Ua_i^+ U^{-1} = \Sigma a_k^+ U_{ki}, \ \check{U} a_i \check{U}^{-1} = \Sigma (U^{-1})_{ik} a_k = \Sigma a_k U_{ki}^{\#}, \tag{7}$$

where $U^{\#}$ is the transpose inverse of $U$. This theorem simply states that the operators $a^+ = \{a^+_i\}$ and $a = \{a_i\}$ transform contragradiently under $U$. As a result the total boson number $N = (a^+ \bullet a)$ is invariant under all $U \in L^{(s)}$. For an orthogonal group $O(s)$, we have $U^{\#} = U$ so that there exist two additional invariants

$$(a^+ \cdot a^+), \ (a \cdot a). \tag{8}$$

This result is of vital importance in constructing the algebraic Hamiltonian for the vibron model.

2) The Jordan-Schwinger operator $\check{U}$ provides a projective representation of the Lie group $L^{(s)}$: Let $U$, $V$ and $W$ be the group elements of $L^{(s)}$ and $UV = W$. Then their Jordan-Schwinger operators satisfy

$$UV = kW, \tag{9}$$

where $k$ is a number called the projective factor for the product of $U$ and $V$. This follows since $UVW^{-1}$ commutes with all the operators $a^+_i$ and $a_i$ on account of Eq. (7) hence it is a constant. For a special case of a unitary group we have

$$|k| = 1, \tag{10}$$

since $U^+ U = V^+ V = W^+ W$.

3) All the theorems stated above on the Jordan-Schwingr representations hold, if we replace the boson operators $\{a^+_i, a_k\}$ by the fermion operators $\{c^+, c_k\}$.

## Algebraic Hamiltonian for Diatomic Molecules

In the vibron model we expand the Hamiltonian of a diato-

mic molecule in terms of the 16 Jordan-Schwinger generators $G_i = \{a^+_m a_n;\ m,n = 1,2,3,4\}$ of the group $U(4)$.

$$H = \Sigma a_i G_i + \Sigma a_{ik} G_{ik} + \cdots \quad (11)$$

It is assumed that $H$ conserves the total vibron number $\hat{N} = (a^+ \cdot a)$ and is invariant under rotations of the subgroup $O(3) \subset U(4)$. For a given total vibron number $N$, the states span the totally symmetric irreducible representations of $U(4)$. Under the Jordan-Schwinger generators $J_1, J_2, J_3$ of $O(3)$,

$$J_i = -i(a^+_j a_k - a^+_k a_j);\ i, j, k = 1, 2, 3 \text{ cyclic} \quad (12)$$

$\pi = (a_1, a_2, a_3)$ and $\pi^+ = (a^+_1, a^+_2, a^+_3)$ transform as vectors while $\sigma = a_4$ and $\sigma^+ = a^+_4$ transform as scalars. Consequently, one can construct three more scalar products

$$\pi^{+2} = (\pi^+ \cdot \pi^+),\ \pi^2 = (\pi \cdot \pi),\ n_\pi = (\pi^+ \cdot \pi). \quad (13)$$

which are consistent with Eq. (8). There exist, however, only three elementary hermitian scalars which conserve the vibron number $\hat{N}$,

$$A = n_\pi,\ B = \pi^{+2}\pi^2,\ C = \pi^{+2}\sigma^2 + \sigma^{+2}\pi^2. \quad (14)$$

Note that $n_\sigma = \sigma^+ \sigma$ is given by $N - n_\pi$.

Now one can write down the most general Hamiltonian, which is a hermitian scalar and conserves $N$, in the form

$$H = H_0 + H_1 + H_2 + \cdots, \quad (15)$$

where $H_n$ is a linear combination of the symmetrized scalars contained in the set $S_n$,

$$S_n = \{[A^{n-2k} B^{k-p} C^p]\};\ n = 0, 1, \cdots,$$

$$k = 0, 1, \cdots, [n/2],\ p = 0, 1, \cdots, k, \quad (16)$$

where $[n/2]$ is the integral part of $n/2$. The set $S_n$ contains the $n$-th order symmetrized scalars with respect to the generators of $U(4)$ and its order $|S_n|$ is given by

$$|S_n| = ([n/2]+1)([n/2]+2). \quad (17)$$

It can be shown[3] that the operators $A$, $B$ and $C$ can be expressed in terms of the Casimir operators belonging to two different group chains. This helps the actual calculation of the spectra. A detailed calculation based on the most general Hamiltonian given in Eq. (15) will be given in a forthcoming paper.

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# Synthesis and Liquid Crystalline Properties of Dimesogenic Compounds Containing Trifluoromethyl Substituents at Terminal Phenylene Rings and Central Decamethylene Spacer

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A series of new dimensogenic compounds whose mesogens are of aromatic ester or amide type having a trifluoromethyl ($CF_3$) substituent at the para-position of each terminal phenolic rings were prepared and their liquid crystalline properties were studied by differential scanning calorimetry (DSC) and on a cross-polarizing microscope. The compounds have two identical mesogenic units bracketing a central decamethylene spacer. Trifluoromethyl group appears to favor the formation of smectic phases when it is attached to a phenoxy or anilide terminal. Its group efficiency for mesophase formation seems to be inferior to other common substituents. A thermodynamic analysis of the phase transitions was made and the results were explained in relation to the structures of the compounds.

## Introduction

Thermotropic behavior of various dimesogenic compounds that consist of two identical mesogenic units bracketing a central spacer has been a subject of our previous reports.[1-6] These compounds exhibits very interesting properties such as odd-even effect in melting ($T_m$) and isotropization temperatures ($T_i$) when the spacer is polymethylene,[7] a zig-zag odd-even effect in the entropy change for isotropization, greater values in thermodynamic parameters of $\Delta H_m$,