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Point symmetries and intrinsic hamiltonians

Symetrie punktowe a hamiltoniany w układzie wewnętrznym

ABSTRACT

In the paper the group algebra formalism, a generalization of the Algebraic Generator Coordinate Method, has been used to relate the quantum numbers labelling the irreducible representations of point groups and the physical quantum numbers required for the irreducible representations of the orthogonal group $O(3)$. Within the formalism, the method of construction of the point-group determined Hamiltonian has been proposed as a general way to analyze the symmetry properties of the molecular, atomic and nuclear energy spectra. An example of C_4 point symmetry actually widely discussed in nuclear physics of exotic states has been shortly analyzed.

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1. INTRODUCTION

Point-symmetries are widely used in physics and chemistry. They allow to determine main features of molecular and atomic spectra [1]. For example, the contemporary high-resolution laser spectroscopy gives a good tool to investigate details of spectra, which can be connected with rotational transitions in complex polyatomic molecules. Making use of point-symmetries allows to relate thousands of these transitions with structure of the molecules. Non-linear dynamics of these objects, constrained by the appropriate symmetries, can also lead to discoveries of new effects, such as “critical phenomenon” in rotational spectra which represents a qualitative change of collective-motion dynamics of the molecule. This phenomenon, often called “bifurcation”, occurs for high values of quantum number I of angular momentum and it is induced by nonlinear effects in the molecule [2].

It seems, that a new field of applications for the point–symmetries is opened in nuclear physics. Recent experimental analyses of the high resolution nuclear spectra with multidetector arrays like EUROGAM have shown the $\Delta I = 4$ bifurcation (or staggering) in the superdeformed bands of some nuclei. It is possible that this bifurcation is due to the existence of a point symmetry C_4 [3,4] – similarly to the situation encountered in molecular physics.

A theoretical analysis of the discrete symmetries in nuclei, based on the average field concept, is not unique and it is dependent on many details of the nuclear dynamics. In this formalism it is not easy to determine the nature of observed staggering. It is very difficult to decide whether the staggering is due to symmetry or is a dynamical effect only. An idea is to consider the appropriate group of theoretical models to get more reliable theoretical interpretation of the observed behaviour of nuclear spectra. For continuous symmetry groups there exists a well known formalism of dynamical symmetries, useful in such an analysis. Within this formalism the Hamiltonians of physical systems are modelled by functions of generators of the groups. In the case of discrete symmetries there are no infinitesimal generators at all. In this paper a possible solution of the problem is proposed by a construction of the model Hamiltonian not from generators (since they do not exist), but from the group elements themselves. As an example, the case of C_4 symmetry will be shortly considered here.

2. THE GROUP ALGEBRAS QM(*G*,*G'*)

We use the group algebra formalism which is a generalization of the Algebraic Generator Coordinate Method (AGCM) [5,6]. This excellent formalism allows to determine the representations of the discrete symmetry groups in the intrinsic frame and translate the results to the laboratory one. It also allows to analyze or even construct the Hamiltonians invariant under a given symmetry group.

Presentation of an elementary theory of the group algebras for finite groups one can find e.g., in [7]. On the other hand, a lot of information about group algebras for continuous groups is contained in [8]. For our purpose we need to introduce a combined structure of two algebras: one for discrete and one for continuous groups. We will denote these algebras by QM(*G*,*G'*), where *G* is a continuous group and *G'* is a discrete subgroup of *G*. In the present case we will focus on $O(3)$ group as a continuous one, but the formalism is quite general and can be used for any compact group. The only assumption about *G'* is that it is a subgroup of *G*.

The algebra QM(*G*,*G'*) (to emphasize universality of this formalism we use the abbreviation $G = O(3)$) is constructed using the sums:

$$S = u + \breve{\alpha}\,, \tag{1}$$

where, u is a function belonging to the space of integrable functions $L^1(G)$ and

$$\breve{\alpha} = \sum_{g\in G'} \alpha(g)g\,. \tag{2}$$

In equation (2), $\alpha(g)$ is a complex function on group G'. Sum and multiplication of elements of this type by a complex numbers are defined in the usual way, but multiplication of the elements is defined by the following relations ($u, v \in L^1(G)$ and $g, g_1, g_2 \in G'$):

$$(u \circ v)g'' = \int_G dg' u(g') v\left(g'^{-1} g''\right), \tag{3}$$

$$g \circ u(g') = u\left(g^{-1} g'\right), \tag{4}$$

$$u(g') \circ g = u\left(g' g^{-1}\right), \tag{5}$$

$$g_1 \circ g_2 = g_1 g_2; \quad \text{multiplication in } G', \tag{6}$$

and the distributive law with respect to the addition. Another available operation in this algebra is involution $^{\#}$, an analog of hermitian conjugation, defined by:

$$\left(u(g) + \sum_{g' \in G'} \alpha(g') g' \right)^{\#} = u^{*}\left(g^{-1}\right) + \sum_{g' \in G'} \alpha^{*}(g') g'^{-1}, \tag{7}$$

One can easily find that the space of complex functions belonging to QM(*G*,*G'*) is a subalgebra, even more, it is an ideal of QM(*G.G'*) which we will denote by QM'(*G*,*G'*). The space of formal sums (2) is also a subalgebra of QM(*G*,*G'*) which we denote by QM''(*G*,*G'*).

The algebra QM(*G*,*G'*) can be represented by the appropriate algebra of operators in the Hilbert space H of physical states. For this purpose one needs to choose the unitary operator representation *T*(*g*) of the group *G* in the Hilbert space H and relate this representation to the elemets of QM(*G*,*G'*) as follows:

$$u + \breve{\alpha} \to \int dg u(g)^{*} T(g) + \sum_{g \in G'} \alpha(g) T(g). \tag{8}$$

However, one needs to realize that the representation described above can be not faithful.

We also need to introduce some special elements of the algebra QM(*G*,*G'*) related to some subgroups of the discrete group *G'*. More generally, let *N* be a group and $\chi_N^{(\Gamma)}$ denotes the irreducible character of *N* [7]. Then

$$\breve{\chi}_N^{(\Gamma)} = \sum_{h \in N} \chi_N^{(\Gamma)}(h)^* h \,. \tag{9}$$

The elements (9) which we call algebraic characters, correspond (up to a normalization constant) to the projection operators projecting onto the appropriate representations of *N*. Similarly, if $D_{a,b}^{(A)*} \in \mathrm{QM}(G, G')$ is a matrix element of an irreducible representation of the group *G* then in the operator representation it corresponds (up to a normalization constant) to the so-called generalized projection operator [9]. Using this representation of QM(*G*,*G'*) one can easily understand the relation between this algebra and representations of the group *G* and its subgroups.

Let $D^{(\kappa,J)}$ denote the matrices of irreducible representations of the $G = O(3) = SO(3) \times C_i$ group, where κ and *J* denote the parity and the total angular momentum quantum numbers, respectively. This representation can be written as a product of representations for *SO*(3) and C_i groups:

$$D_{M,K}^{(\kappa,J)}(s,\Omega) = \chi_{C_i}^{(\kappa)}(s) D_{MK}^{J}(\Omega), \tag{10}$$

where $s \in C_i$, $\Omega \in SO(3)$, $\chi_{C_i}^{(\kappa)}(s)$ is an irreducible character of C_i and $D_{MK}^{J}(\Omega)$ is the standard Wigner function for *SO*(3). By the Peter–Weyl theorem [9] one can expand $D_{M,K}^{(\kappa,J)}(g)$, where $(s,\Omega) = g \in G'$, into the matrices of irreducible representations of *G'* group

$$D_{M,K}^{(\kappa,J)}(g) = \sum_{\Gamma\alpha\beta} c_{(\Gamma)\alpha\beta}^{(\kappa,J)MK} \Delta_{\alpha\beta}^{(\Gamma)}(g), \tag{11}$$

for all $g \in G'$. Here $\Delta^{(\Gamma)}$ denotes an irreducible representation of the group *G'*. On the other hand

$$D_{M,K}^{(\kappa,J)*} \circ \breve{\Delta}_{\alpha\beta}^{(\Gamma)}(g) = \sum_{M'} \left\{ \sum_{g \in G'} D_{KM'}^{(\kappa,J)}(g) \Delta_{\alpha\beta}^{(\Gamma)*}(g) \right\} D_{MM'}^{(\kappa,J)*}, \tag{12}$$

where $\breve{\Delta}^{(\Gamma)}_{\alpha\beta}(g)=\sum_{g\in G'}\Delta^{(\Gamma)*}_{\alpha\beta}(g)\,g$. Using eq. (11) one can demonstrate that

$$\sum_{g\in G'} D^{(\kappa,J)}_{KM'}(g)\Delta^{(\Gamma)*}_{\alpha\beta}(g)=\frac{\mathrm{card}(G')}{\dim(\Gamma)}c^{(\kappa,J)KM'}_{(\Gamma)\alpha\beta}, \tag{13}$$

where card(G') is the order of the discrete group G' and dim(Γ) denotes the dimension of i.r. $\Delta^{(\Gamma)}$. A combination of (13) and (12) gives the following decomposition within the algebra QM(G,G')

$$D^{(\kappa,J)*}_{MK}\circ\breve{\Delta}^{(\Gamma)}_{\alpha\beta}=\frac{\mathrm{card}(G')}{\dim(\Gamma)}\sum_{M'}c^{(\kappa,J)KM'}_{(\Gamma)\alpha\beta}D^{(\kappa,J)*}_{MM'} \tag{14}$$

which allows to determine the relations between i.r. of G and G'. The formula (14) requires knowledge of the i.r. for G' and in many cases it is not too useful. However, summing over $\alpha=\beta$ one can get more convenient expression which allows to show which representations of G' are present in the vectors (10) representing basis of i.r. of $G=O(3)$. This expression requires only the irreducible characters of the group G':

$$D^{(\kappa,J)*}_{MK}\circ\breve{\chi}^{(\Gamma)}_{G'}=\frac{\mathrm{card}(G')}{\dim(\Gamma)}\sum_{M'}c^{(\kappa,J)KM'}_{(\Gamma)}D^{(\kappa,J)*}_{MM'}. \tag{15}$$

This basic formula gives us relations between the quantum numbers Γ labelling the i.r. of G' and the laboratory quantum numbers κ (parity), J (total angular momentum) and K the projection of the total angular momentum onto intrinsic "z" axis of the physical system under consideration. If for a given κ, J and K, $D^{(\kappa,J)*}_{MK}\circ\breve{\chi}^{(\Gamma)}_{G'}$ is equal zero for all M, the state (10) cannot contain any vector belonging to the carrier space of the representation $\Delta^{(\Gamma)}$ of G'.

Useful information is contained also in the multiplicity coefficients showing how many times a given i.r. of the group G' is contained in a given i.r. of the group $G=O(3)$:

$$c_{(\Gamma)}^{(\kappa,J)} = \sum_{K,\alpha} c_{(\Gamma)\alpha\alpha}^{(\kappa,J)KK} \qquad (16)$$

in the decomposition of i.r. according to the group chain

$$G \supset G' \qquad (17)$$

The decomposition can be written as the orthogonal sum:

$$D^{(\kappa,J)} = \bigoplus_{\Gamma} c_{(\Gamma)}^{(\kappa,J)} \Delta^{(\Gamma)} \qquad (18)$$

and the multiplicity coefficients can be expressed as:

$$c_{(\Gamma)}^{(\kappa,J)} = \frac{\dim(\Gamma)}{\mathrm{card}(G')} \sum_{g \in G'} \chi_{O(3)}^{(\kappa,J)}(g) \chi_{G'}^{(\Gamma)*}(g) . \qquad (19)$$

In the case of $O(3)$ group, which is considered here, these are just the appropriate Clebsch coeficients.

3. HAMILTONIANS GENERATED BY THE POINT GROUPS

In the case of discrete groups the standard Lie group methods of constructing of the Hamiltonians from infinitesimal generators is useless. Instead we propose here the construction of the model Hamiltonians from the group elements themselves. In the following we restrict ourselves to the algebra QM(G,G'), where $G = O(3)$ and $G' \in G$ is a point symmetry group. This restriction can be overcome easily.

According to the theorem by Burnside [13] within the carrier space L_π of the unitary irreducible representation (π, L_π), for every linear operator S defined in L_π there exist a series of numbers $c_1, c_2, ..., c_n$ and the elements g_1, s$g_2, ..., g_n \in G$ such that

$$S = \sum_{k=1}^{n} c_k \pi(g_k). \tag{20}$$

This means that every Hamiltonian which does not mix the irreducible representations of the group G' can be, in some way, expressed in terms of operators (20) with coefficients c_k dependent on characteristics ν of equivalent representations of G'. The quantum numbers ν depend on structure of the physical system under consideration and can distinguish equivalent irreducible representations of G'. As a consequence the space of physical states H e.g., the many-body space of states of a nuclear system, can be decomposed into an orthogonal sum of subspaces H_ν spanned by the states with the same set of quantum numbers ν.

The most interesting from the physical point of view are Hamiltonians invariant under a given point symmetry group G'. These Hamiltonians can be expressed in terms of the operators (20) as building blocks. To show the construction of the Hamiltonian with the symmetry group G' in terms of the group algebra QM(G,G') one needs to consider the center N of the algebra i.e., the set of elements commuting with all other algebra elements. One can see that all elements of N can be obtained in the following form:

$$\tilde{X} = \sum_{g \in V_n}^{n} g\,, \tag{21}$$

where V_n denotes the n-th class of conjugated elements of the group G'. The number of classes NC(G') is equal to the number of non-equivalent irreducible unitary representations which, in turn, allow to distinguish different energy levels of the Hamiltonian symmetric under the group G'. From the above, one can conclude that in the carrier subspace of set (with fixed ν) of non-equivalent irreducible representations the most general form of G' invariant Hamiltonian is given by the formula:

$$H_{G'}(\nu) = \sum_{k=1}^{\mathrm{NC}(G')} \gamma_k \tilde{X}_k\,, \tag{22}$$

where the coupling constants $\gamma_k(\nu)$ are, in general, complex functions dependent on a set of quantum numbers ν, invariant under *G'*, fulfilling the hermiticity condition for $H_{G'(\nu)}$:

$$H_{G'(\nu)} = H_{G'}(\nu)^2 = \sum_{k=1}^{NC(G')} \gamma_k^* \sum_{g \in V_n} g^{-1} . \tag{23}$$

In fact, in equation (22), for fixed quantum numbers ν the elements $\tilde{X}_k$ should be replaced by their representatives in the appropriate subspaces H_ν. However, making use of the GNS construction one can always embed the space H_ν into the unique model space independent of ν and constructed on a purely algebraic level. All dependence on quantum numbers ν enters only through the coupling constants $\gamma_k(\nu)$.

Let us denote by

$$|\nu; \Gamma\alpha\rangle \tag{24}$$

an orthonormal basis in H, where [Γ] label the irreducible unitary representations of *G'* and *a* distinguishes the vectors within these representations. Because of tensor nature of (24), with respect to group *G'*, the action of *G'* on (24) can be obviously written as:

$$g|\nu; \Gamma\alpha\rangle = \sum_{\alpha'} \Delta^{\Gamma}_{\alpha'\alpha}(g)|\nu; \Gamma\alpha'\rangle . \tag{25}$$

where $\Delta^{\Gamma}_{\alpha'\alpha}(g)$ are the appropriate matrix elements of the irreducible unitary representation of the group *G'*.

The physical states (24) allow to define the following positive functional in the appropriate algebra of operators defined in the state space of our physical system:

$$\langle \nu; A\rangle = \sum_{\Gamma} p_\Gamma \frac{1}{\dim[\Gamma]} \sum_{\alpha} \langle \nu; \Gamma\alpha | A | \nu; \Gamma\alpha\rangle , \tag{26}$$

where A is the operator, $p_\Gamma = (\dim[\Gamma])^2 / \mathrm{card}(G')$, $\dim[\Gamma]$ denotes the dimension of the representation [Γ] and card(U) gives the number of element in the set *U*. The functional (26) determines the metastate on the algebra QM(*G*,*G'*) with the metastate kernel:

$$\langle \nu; g \rangle = \sum_{\Gamma} p_\Gamma \frac{1}{\dim[\Gamma]} \chi_{G'}^{(\Gamma)}(g), \tag{27}$$

where $\chi_{G'}^{(\Gamma)}$ denotes the irreducible character of the representation [Γ]. For further purpose we need to calculate the action of (21) onto (24). After some transformations we get:

$$\tilde{X}_n |\nu; \Gamma\alpha\rangle = \sum_{\alpha} [\sum_{g \in V_n} \Delta^{\Gamma}_{\alpha'\alpha}(g)] |\nu; \Gamma\alpha'\rangle. \tag{28}$$

One can also find that the matrix

$$\Delta_n^{\Gamma} = \sum_{g \in V_n} \Delta^{\Gamma}(g) \tag{29}$$

commutes [7 § 3.17] with all other matrices of the representation [Γ]. According to well known Schur's lemmas the matrix (29) must be proportional to unity:

$$\Delta_n^{\Gamma} = \lambda_n \mathbf{I}, \tag{30}$$

where

$$\lambda_n = \frac{\mathrm{card}(V_n)}{\dim[\Gamma]} \chi_{G'}^{(\Gamma)}(\dot{g}_n) \tag{31}$$

and $\dot{g}_n \in V_n$ is a representative of the class V_n.

Using the last three relations one can get a very simple result:

$$\tilde{X}_n \left| \nu; \Gamma\alpha \right\rangle = \frac{\mathrm{card}(V_n)}{\dim[\Gamma]} \chi_{G'}^{(\Gamma)}(\dot{g}_n) \left| \nu; \Gamma\alpha \right\rangle \tag{32}$$

Equation (32) and the orthogonality relation for irreducible characters [7] allow to show the orthogonality of the elements (21) with respect to the metastate (26):

$$\left\langle \nu; \tilde{X}_m^{\#} \circ \tilde{X}_n \right\rangle = \mathrm{card}(V_n)\delta_{mn} . \tag{33}$$

Normalization of $\tilde{X}_n$

$$X_n = \frac{1}{\sqrt{\mathrm{card}(V_n)}} \tilde{X}_n \tag{34}$$

leads to the set of orthonormal operators (elements) in both the algebra QM(G,G') and the algebra of operators in the space of physical states with respect to the scalar product generated by the metastate:

$$\left(A \middle| B\right)_\nu = \left\langle \nu; A^{\#} \circ B \right\rangle, \tag{35}$$

where $^{\#}$ denotes either involution operation in the algebra QM(G,G') or the hermitian conjugation in the space H.

Now we are in a position to express the physical Hamiltonian H in the space spanned by the set of orthonormal operators (34) providing the scalar product in the form (35). The standard expansion procedure leads to the formula:

$$H \to H_{G'(\nu)} = \sum_{n}^{\mathrm{NC}(G')} \left(\mathrm{X_n} \middle| H\right)_\nu X_n . \tag{36}$$

Straightforward but slightly longer calculations give the coupling constants in the following form:

$$\gamma_n(\nu) = (\mathrm{card}(V_n))^{-\frac{1}{2}} \left\langle \nu; X_n^{\blacksquare} H \right\rangle = \\ = \frac{1}{\mathrm{card}(G')} \sum_{\Gamma} \chi_{G'}^{(\Gamma)} (\dot{g}_n)^* \sum_{\alpha} \left\langle \nu; \Gamma\alpha \middle| H \middle| \nu; \Gamma\alpha \right\rangle . \tag{37}$$

In formula (37) we do not use the property that the Hamiltonian H is invariant under group G'. Making use of the invariance properties, the formula for the coupling constants can be simplified after summing over quantum numbers a:

$$\gamma_n(\nu) = \frac{1}{\mathrm{card}(G')} \sum_{\Gamma} \dim[\Gamma] \chi_{G'}^{(\Gamma)} (\dot{g}_n)^* \left\langle \nu; \Gamma\alpha_0 \middle| H \middle| \nu; \Gamma\alpha_0 \right\rangle \tag{38}$$

with an arbitrary but fixed a_0, for every representation $[\Gamma]$.

The expansion (36) is quite general, giving an approximation of the Hamiltonian H within the space H_ν. However, if the states (24) are the eigenstates of the Hamiltonian H invariant under the group G' the expansion is exact. In this case the coupling constants obtained from the formula (38) can be written as:

$$\gamma_n(\nu) = \frac{1}{\mathrm{card}(G')} \sum_{\Gamma} \dim[\Gamma] E(\nu, \Gamma) \chi_{G'}^{(\Gamma)} (\dot{g}_n)^* \tag{39}$$

and the group generated Hamiltonian H_ν can be rewritten in the form of the spectral theorem:

$$H_{G'}(\nu) = \sum_{\Gamma} E(\nu, \Gamma) P^{(\Gamma)} , \tag{40}$$

where

$$P^{(\Gamma)} = \frac{\dim(\Gamma)}{\mathrm{card}(G')} \sum_{n=1}^{\mathrm{NC}(G')} \chi_{G'}^{(\Gamma)} (\dot{g}_n)^{\#} X_n \tag{41}$$

is the projecting operator which projects onto the space of the irreducible representation [Γ]. For fixed ν i.e., within the space H_ν, the Hamiltonians H and $H_{G'}(\nu)$ have the same spectra and eigenvectors.

4. EXAMPLE OF USE OF THE FORMALISM – C_4 SYMMETRY

We would like to illustrate the formalism presented above by the algebra QM(O(3), C_4) [11] in a molecular physics context.

The proper C_4 symmetry can be regarded as a π/2-rotational symmetry in respect to a given fixed axis. In the following we assume z-axis to be the four-fold symmetry axis. This is a simplest choice of the reference frame. The C_4-group is an abelian and cyclic group of fourth order, and therefore it has four one-dimensional irreducible representations. They can be labelled by a single quantum number Γ = μ = 0, 1, 2, 3. The corresponding irreducible characters can be written as

$$P^{(\mu)}_{C_4}((C_4)^n) = i^{\mu n} , \tag{42}$$

where C_4 (not to be confuced with C_4) is a generator of $G' = C_4$ group and ν may take the values 0, 1, 2 and 3.

First of all, we can calculate the multiplicity coefficients in the decompositon (16) using (19) and (42). After a short derivation one can obtain

$$c^{(\kappa, J)}_{(\mu)} = \frac{1}{4}\sum_{n=0}^{3}\sum_{M=-J}^{J} e^{-in(M+\mu)\frac{\pi}{2}} . \tag{43}$$

The coeffcients for the angular momenta J = 0, ... ,20 are shown in the Table 1.

Table 1. The multiplicity coefficients in decomposition of irreducible representations of $O(3)$ group into irreducible representations of C_4
Współczynniki krotności rozkładu nieprzywiedlnych reprezentacji grupy $O(3)$ w nieprzywiedlne reprezentacje grupy C_4

J	$c_{\mu=0}^{(\kappa,J)}$	$c_{\mu=1}^{(\kappa,J)}$	$c_{\mu=2}^{(\kappa,J)}$	$c_{\mu=3}^{(\kappa,J)}$
1	1	1	0	1
2	1	1	2	1
3	1	2	2	2
4	3	2	2	2
5	3	3	2	3
6	3	3	4	3
7	3	4	4	4
8	5	4	4	4
9	5	5	4	5
10	5	5	6	5
11	5	6	6	6
12	7	6	6	6
13	7	7	6	7
14	7	7	8	7
15	7	8	8	8
16	9	8	8	8
17	9	9	8	9
18	9	9	10	9
19	9	10	10	10
20	11	10	10	10

In the case of abelian groups the basic formula (15) is identical with the one in (14). It can be easily calculated and one can find that

$$D_{MK}^{(\kappa,J)} \circ \breve{\chi}_{C_4}^{(\mu)} = \left\{ \sum_{n=0}^{3} e^{-in(\mu+K)\frac{\pi}{2}} \right\} D_{MK}^{(\kappa,J)*} = \begin{cases} 4, & \text{if} \quad \mu + K = 0 \pmod 4 \\ 0, & \text{otherwise} \end{cases}. \qquad (44)$$

From the expression (43) we also get the following relation between the intrinsic quantum number μ and the projection of the angular momentum onto the intrinsic axis K as it is shown in the Table 2.

Table 2. The relation between intrinsic and laboratory quantum numbers C_4
Zależności między liczbami kwantowymi grupy C_4 w układach wewnętrznym i laboratoryjnym

μ	K
0	0, ±4, ±8, ±12
1	..., -5, -1, 3, 7, ...
2	..., -6, -2, 2, 6, ...
3	..., -7, -3, 1, 5, ...

For a given representation $\Delta^{(\mu)}$ of the group C_4 allowed angular momenta J are given by the obvious condition $J \geq |K|$, and the results are independent of parity. The relations for small J, where there are some irregularities, we have listed in the Table 3.

Table 3. Details of the decomposition of irreducible representations of $O(3)$ group into irreducible representations of C_4 for small angular momenta J
Przykłady wybranych rozkładów nieprzywiedlnych reprezentacji grupy $O(3)$ na nieprzywiedlne reprezentacje grupy C_4

J	μ	K
0	0	0
	1	-
	2	-
	3	-
1	0	0
	1	-1
	2	-
	3	1
2	0	0
	1	-1
	2	-2.2
	3	1

We define the intrinsic Hamiltonian for C_4 symmetry in terms of group elements. Taking into account that C_4 is an abelian group implies that all the sums in (21) consist of a single term. From equation (22) one can obtain the Hamiltonian invariant under this symmetry as:

$$\breve{H}_{C_4}(\nu) = \gamma_0(\nu) e_G + \gamma_1(\nu) C_4 + \gamma_2(\nu)(C_4)^2 + \gamma_3(\nu)(C_4)^3 . \qquad (45)$$

In the following we assume that the coupling constants $\gamma_n(\nu)$ fulfil the conditions: γ_0 and γ_2 are real numbers, $\gamma_3 = \gamma_1^*$, and generally can be complex. These conditions are required to make the operator (45) selfconjugated (hermitian) with respect to involution (23).

The energy spectrum can be easily calculated from the resolvent of $\breve{H}_{C_4}$:

$$\left(Ee_G - \breve{H}_{C_4}\right)^{-1} \qquad (46)$$

using the base $\breve{\chi}_{C_4}^{(\mu)}$ defined by (9). For the i.r. $\Delta^{(\mu)}$ the eigenenergies are given by:

$$E(\mu) = \gamma_0 + \gamma_1'[1 + (-1)^\mu](1 - \mu) + \gamma_1''[1 - (-1)^\mu](\mu - 2) + \gamma_2(-1)^\mu , \qquad (47)$$

where $\gamma_1' = \mathrm{Re}\,\gamma_1$ and $\gamma_1'' = \mathrm{Im}\,\gamma_1$.

Using the GNS procedure [12], one can construct the space of states for the Hamiltonian (45). However it is not required in our analysis.

Hamiltonian defined by (45) is related to the many-body Hamiltonian by $\gamma_n(\nu)$ coefficients which are obtained from (38). For C_4 type symmetry these state-dependent coupling constants can be expressed in the following form:

$$\gamma_n(\nu) = \frac{1}{16}\sum_{m=0}^{3} \chi_{C_4}^{(m)}\left(C_4^n\right)^* \left[\sum_{n_3}^{3} \chi_{C_4}^{(m)}\left(C_4^{n_3}\right)^* \left\langle \nu \right| (C_4)^{n_3} \left| \nu \right\rangle\right]^{-1} \sum_{n_1,n_2}^{3} \chi_{C_4}^{(m)}\left(C_4^{n_1+n_2}\right)^* \left\langle \nu \right| (C_4)^{n_1} H (C_4)^{n_2} \left| \nu \right\rangle, \qquad (48)$$

where $\{|\nu\rangle\}$ denotes a family of the generating states in the many-body space K. These states are projected onto i.r. of C_4 spanned by the states of the form (24).

Summation in (47) is carried out over all i.r. of C_4 for which

$$\sum_{n_3=0}^{3} \chi_{C_4}^{(m)}\left(C_4^{n_3}\right)^* \left\langle \nu \right| (C_4)^{n_3} \left| \nu \right\rangle \neq 0. \qquad (49)$$

Of course, the state dependent Hamiltonian $\breve{H}_{C_4}$ is able to reproduce the energy spectrum of the original many-body Hamiltonian H. If Hamiltonian H is invariant under C_4 transformations and, in addition, the generating states $|\nu\rangle$ are its eigenstates, according to (39), formula (48) reduces to much simpler form

$$\gamma_n(\nu) = \frac{1}{4} H(\nu) \sum_{m=0}^{3} \chi_{C_4}^{(m)} \left(C_4^n\right)^* = H(\nu)\delta_{n0} . \tag{50}$$

As a result we have obtained a procedure which allows to analyze an influence of exact or approximate C_4 symmetry onto a physical system described by a Hamiltonian H. The state dependent coupling constants $\gamma_n(\nu)$ determine a form of the spectrum of physical system within a cluster of states generated from the many-body state $|\nu\rangle$ by the projections onto different irreducible representations of the C_4 group.

In practice, we need to use an approximate scheme, usually based on the mean field approach. Let the physical system be described by the mean field Hamiltonian H_0 with the appropriate corrections, responsible for the smooth, regular part of the energy spectrum plus the term H' representing small perturbation and invariant under C_4 symmetry.

As a result the total Hamitonian H is invariant under transformations from C_4 group:

$$H = H_0 + H'. \tag{51}$$

We represent this Hamiltonian by the group-generated Hamiltonian $\breve{H}_{C_4}$ which also splits into the two terms. Denoting by $E_0(\nu)$ and $|\nu\rangle$ the eigenenergies and the corresponding eigenstates of H_0, the eigenenergies of $\breve{H}_{C_4}$ can be analytically calculated and are given by:

$$\begin{aligned} E(\mu,\nu) = E_0(\nu) + \gamma_0(\nu;H') + \gamma_1'(\nu;H')[1+(-1)^{\mu}](1-\mu) + \\ + \gamma_1''(\nu;H')[1-(-1)^{\mu}](\mu-2) + \gamma_2(\nu;H')(-1)^{\mu} , \end{aligned} \tag{52}$$

where $\gamma_n(\nu;H')$ denote the coupling constants (48) calculated for H'. The formula can be rewritten in a manner which shows a possible staggerring in the spectrum. The staggering which can be found here is, generally, due to C_4 symmetry. It is not a dynamical effect caused by a special properties of the interactions. To see this effect one needs to consider two cases. The first one corresponds to even representations i.e. of $\mu = 0, 2$ of C_4. It is more interesting because it is possibly able to describe the experimental observations for some superdeformed nuclei. In this case we get the $\Delta I = 4$ staggering within the bands with positive parity and even angular momenta

$$E(\mu,\nu) = E_0(\nu) + \gamma_0(\nu;H') + \gamma_2(\nu;H') + \begin{cases} 2\gamma_1'(\nu;H'), & \mu = 0; \\ -2\gamma_1'(\nu;H'), & \mu = 2. \end{cases} \quad (53)$$

For odd representations, $\mu = 1, 3$, one can obtain a similar result

$$E(\mu,\nu) = E_0(\nu) + \gamma_0(\nu;H') - \gamma_2(\nu;H') + \begin{cases} -2\gamma_1''(\nu;H'), & \mu = 1; \\ 2\gamma_1''(\nu;H'), & \mu = 3. \end{cases} \quad (54)$$

One needs to emphasize once again that the coupling constants gamma are state dependent. Their values depend on the actual form of both parts of the physical Hamiltonian (51). The quantum numbers of physical system can be easily related to the label μ, what is given in the Table 2.

5. FINAL REMARKS

In the paper we have shown a scheme of a useful algebraic formalism. We have illustrated it by an example of C_4 symmetry. The formalism can be applied to any arbitrary discrete group, which makes it quite useful. As it was shown in the last paragraph the formalism can be also applied to the effective analysis within the approximate theory like mean field approach. It is enough to extract from the total effective Hamiltonian or the other more phenomenological procedure the parts responsible for the mean field describing a smooth part of the energy spectra and the additional (usually small) terms with the appropriate symmetry treated as a perturbation. The example shows clearly the effect of such procedure – a kind of staggering in the energy spectra due to the symmetry C_4.

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STRESZCZENIE

W niniejszej pracy użyto formalizmu algebraicznego – będącego uogólnieniem metody współrzędnej generującej (AGCM) – do wyprowadzenia związków między liczbami kwantowymi znakującymi nieprzywiedlne reprezentacje grup punktowych a fizycznymi liczbami kwantowymi, związanymi z nieprzywiedlnymi reprezentacjami ortogonalnej grupy $O(3)$. Umożliwia to konstrukcję hamiltonianów nie tylko z generatorów grupy ciągłej, ale także z elementów grup dyskretnych, co umożliwia opisanie szerokiej klasy symetrii.

We wstępie przedstawiono nowe wyniki eksperymentalne, przy uzyskaniu których formalizm algebraiczny może być użyteczny. Rozdział drugi zawiera przegląd głównych zało-

żeń metody AGCM oraz przyk grupy $O(3)$. W rozdziale trzecim opisano metodę budowy y dyskretnej na podstawie rozszerzonej metody AGCM. Kolejny rozdział zawiera przykład użycia formalizmu w przypadku grupy dyskretnej C_4.