ISSN 0029 - 3865

CBPF-NF-021/87

ON THE LABELING AND SYMMETRY ADAPTATION OF THE SOLVABLE FINITE GROUPS REPRESENTATIONS

by

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A B S T R A C T

We propose a method to simultaneously perform a symmetry adaptation and a labeling of the bases of the irreducible representations of the solvable finite groups. It is performed by defining a self-adjoint operator with eigenvalues which evidence the descent in symmetry of the group-subgroups sequences.

We also prove two theorems on the canonicity of the composition series of the solvable groups.

Key-words: Finite groups; Labeling of energy labels.

I. INTRODUCTION

Group theory is a powerful tool for the study of the physical properties of quantum mechanical systems. In order to exploit effectively the symmetry properties of the systems, it is of great importance to know how to perform an adaptation of the corresponding state vectors . In this paper we show that it is possible to make a symmetry adaptation and simultaneously a labeling of the bases of the irreducible representations (irreps) of the finite groups associated to physical problems.

In Section II we show that a composition series of a solvable group is always a canonical sequence, an essential requirement for the labeling to be unique. This is a highly desired result since the majority of the groups associated to solid state physics and quantum chemistry problems are solvable groups - as is the case of crystallographic groups, point groups, Shubnikov groups, etc.

In that section we also show that the sequences of the maximal subgroups of crystallographic point groups are canonical series.

The labeling of the basis functions of the head group in a sequence is perform in Section III, where we show that it is possible to construct a self-adjoint operator for each one of the sequences of the type $\mathbb{G}_0 \supset \mathbb{G}_1 \supset \ldots \supset \mathbb{G}_\ell$, such that the eigenvalues show the descent in symmetry in the chain and their corresponding eigenvectors actually may be the symmetry adapted bases of the irreps.

The key of the labeling consists essentially in adopting the general Bethe's convention for the irreps, such that we let the eigenvalues of the operator be integer numbers given in a convenient form to label the irreps of each group in the sequence. We also show in section III that in order to construct the labeling operators, we only need a character table of the groups envolved in the sequence.

The extension of the method to label the bases of vector fields is analised in section IV where we also propose a solution for the cubic harmonics, that is, the labeling of the bases for the sequence SU(2) $\supset O_h^* \supset \ldots$.

II. CANONICAL SEQUENCES

First we recall that a group has a canonical sequence when the number of times the irreps of each subgroup in the series occur in the restriction of the representations of the corresponding preceding group is either one or zero.

Let a subclass of $g \in \mathbf{G}$ be the set of elements $\{hgh^{-1} | h \in \mathbf{H}\}$, where $\mathbf{H} \subset \mathbf{G}$. Wigner (1968) has shown that if all the subclasses so defined commute, $\mathbf{G} \supset \mathbf{H}$ is a canonical sequence. Since the application of this theorem is in general very difficult, we are going to show that i) $\mathbf{H} \subset \mathbf{G}$ is a canonical sequence if the index of $\mathbf{H}$ in $\mathbf{G}$ satisfies $|\mathbf{G} : \mathbf{H}| \leq 3$ or $|\mathbf{G} : \mathbf{H}| = 4$ in the special case when

$$\mathbf{H}_{\mathbf{G}}^{core} = \bigcap_{g \in \mathbf{G}} g\mathbf{H}g^{-1} \subseteq Z(\mathbf{G}), \tag{1}$$

being $Z(\mathbf{G})$ the group of the center of $\mathbf{G}$, and that ii) every composition series of a solvable group is a canonical sequence. For this purpose, let γ be an irrep of $\mathbf{H}$, Γ an irrep of $\mathbf{G}$ and $\langle\Gamma|\gamma\rangle$ the number of times the representation γ occurs in the restriction $\Gamma_{\mathbf{H}}$ of the representation Γ.
i) From the orthogonality of the characters of the representations of $\mathbf{H}$ and $\mathbf{G}$ we have

$$\sum_{\gamma} \langle\Gamma|\gamma\rangle^2 = (1/|\mathbf{H}|) \sum_{h \in \mathbf{H}} |\chi^{\Gamma}(h)|^2 \quad ,$$

$$\leq (1/|H|) \sum_{g \in G} |\chi^{\Gamma}(g)|^2 = |G|/|H| \quad . \tag{2}$$

Therefore, $\langle \Gamma | \gamma \rangle \leq 1 \quad \forall \quad |G : H| \leq 3$.

It is clear that if G is an abelian group, $H \subset G$ is canonical. Then, let us suppose that G is not abelian and that H and G are groups such that if $H \subset G$ equation (1) holds, i.e., the core of H in G is contained in the group of the center of G. Under this assumption, we shall now prove that

$$\sum_{h \in H} |\chi^{\Gamma}(h)|^2 < |G| \quad .$$

If we suppose that in equation (2) the equality holds, we should have $\chi^{\Gamma}(g) = 0 \quad \forall \quad g \in (G - H_G^{core})$. Then, equation (2) might become

$$\sum_{g \in G} |\chi^{\Gamma}(g)|^2 = |H_G^{core}|(\chi^{\Gamma}(1))^2 = |G| \; , \tag{3}$$

and if we sum $(\chi^{\Gamma}(1))^2$ over all $\Gamma \in$ irrep(G), we again obtain $|G|$. Therefore,

$|H_G^{core}|$ = number of conjugacy classes of G.

Clearly, the resulting equality contradicts the assumption because since G is not abelian, the number of classes of G should be greater than the order of $Z(G)$. We then conclude that if $|G:H| = 4$ and $H_G^{core} \subseteq Z(G)$, the sequence $H \subset G$ is canonical. When G is a crystallographic point group, we have $|G_i : G_{i+1}| = 2$, 3 or 4 for the maximal subgroups sequences. This index is equal to 4 for the sequences $O_h^* \supset D_{3h}^*$, $O^* \supset D_3^*$, $T_d^* \supset C_{3v}^*$, $T_h^* \supset C_{3h}^*$. Equation (1) holds for all these sequences and therefore, the sequences of maximal subgroups of crystallographic point groups are canonical.

ii) Let the stabilizer of γ in G be given by

$$S_{\mathbf{G}}(\gamma) = \{g\epsilon\mathbf{G} \mid \gamma^g(h)=\gamma(ghg^{-1})\sim\gamma(h)\} \quad \forall\ h\epsilon\mathbf{H},$$

being $\mathbf{H}$ a normal subgroup of $\mathbf{G}$.

According to this,

$$\mathbf{H} \subset S_{\mathbf{G}}(\gamma) \subset \mathbf{G} \quad , \tag{4}$$

and we can decompose $\mathbf{G}$ into cosets of $S_{\mathbf{G}}(\gamma)$.

If $t_1, \ldots, t_\ell$ are the representatives of the cosets, with $t_1=1$ and $\ell = |\mathbf{G}|/|S_{\mathbf{G}}(\gamma)|$, $\mathbf{H}$ has ℓ different conjugate irreps given by

$$\gamma_k(h) = \gamma(t_k\ h\ t_k^{-1}) \quad .$$

Since $\langle\Gamma|\gamma\rangle = (1/|\mathbf{H}|) \sum_{h\epsilon\mathbf{H}} \chi^\Gamma(h)\ \chi^\gamma(h)^*$,

and $\qquad \chi^\Gamma(ghg^{-1}) = \chi^\Gamma(h)$,

we have $\quad \langle\Gamma|\gamma_k\rangle = \langle\Gamma|\gamma\rangle \quad$ for $\quad k = 1, \ldots, \ell$.

In order to show that the restriction $\Gamma_{\mathbf{H}}$ contains only the irreps γ_k , we induce the representation $\gamma^{\mathbf{G}}$ from $\gamma \in$ irrep($\mathbf{H}$) .

From Frobenius reciprocity theorem, and assuming $\langle\Gamma|\gamma\rangle\neq 0$, it is clear that $\Gamma \in$ irrep($\mathbf{G}$) occurs in this induced representation, and since the character of $\gamma^{\mathbf{G}}$ can be given by

$$\chi^{\gamma^{\mathbf{G}}}(h) = \sum_{i=1}^{\ell} \chi^\gamma(t_i\ h\ t_i^{-1})$$
$$= \sum_{i=1}^{\ell} \chi^{\gamma_i}(h) ,$$

we conclude that the γ_i are the only irreps contained in $\Gamma_{\mathbf{H}}$.

Then, we can write

$$\chi^{\Gamma}(h) = \langle\Gamma|\gamma\rangle \sum_{i=1}^{\ell} \chi^{\gamma i}(h),$$

and from the orthogonality of the characters we have

$$\sum_{\gamma} \langle\Gamma|\gamma\rangle^2 = \sum_{i=1}^{\ell} \langle\Gamma|\gamma_i\rangle^2$$

$$= \langle\Gamma|\gamma\rangle^2 \; |\mathbf{G}|/|S_{\mathbf{G}}(\gamma)|$$

$$= (1/|\mathbf{H}|) \sum_{h\in\mathbf{H}} |\chi^{\Gamma}(h)|^2 \;\le\; |\mathbf{G}|/|\mathbf{H}| \; .$$

It then follows that

$$\langle\Gamma|\gamma\rangle^2 \le |S_{\mathbf{G}}(\gamma)|/|\mathbf{H}| \quad . \tag{5}$$

Now, if the invariant subgroup $\mathbf{H}$ of $\mathbf{G}$ is such that $|\mathbf{G}/\mathbf{H}| = p$ (a prime number), from equation (4) we have that either $S_{\mathbf{G}}(\gamma) = \mathbf{H}$ or $S_{\mathbf{G}}(\gamma) = \mathbf{G}$.

In the first case, equation (5) yields $\langle\Gamma|\gamma\rangle = 1$ and consequently

$$\Gamma(h) = \sum_{i=1}^{p} \gamma_i(h).$$

Therefore, $\chi^{\Gamma}(g) = 0 \quad \forall \; g \in (\mathbf{G} - \mathbf{H})$ is a necessary condition for $S_{\mathbf{G}}(\gamma) = \mathbf{H}$. But it is also a sufficient condition because if $S_{\mathbf{G}}(\gamma) = \mathbf{G}$, there would be at least one conjugation class C of $\mathbf{G}$ contained in $(\mathbf{G} - \mathbf{H})$ such that $\chi^{\Gamma}(C) \neq 0$. But if $\chi^{\Gamma}(g) = 0 \quad \forall \; g \in (\mathbf{G} - \mathbf{H})$, the equality holds in equation (5) and therefore $\langle\Gamma|\gamma\rangle^2 = p$ in contradiction with our assumption that p is a prime number.

Since by hypothesis $\mathbf{G}/\mathbf{H} \sim C_p$, there are in $\mathbf{G}$ at least p one-dimensional representations λ_n of the form $\lambda_n(t^k H) = \omega^{nk}$, with $\omega^p=1$ and where t is the representative of the coset of **H** in **G** . Since we know that the characters of the irrep Γ of **G** [for $S_G(\Gamma)=G$] are different from zero for at least one class $C \subset (G - H)$, we have that there are in **G** at least p non-equivalent irreps Γ_n related by

$$\Gamma_n(t^k h) = \lambda_n(t^k H)\ \Gamma_p(t^k h)$$

$$= \omega^{nk}\ \Gamma_p(t^k h)\ ,\quad \forall\ \ h\in H\ ,\ 0<n<p\ \text{ and }\ \Gamma_p \equiv \Gamma\ .$$

From this, the orthogonality relations for the irreps of **G** can be written in the form

$$\sum_{h\in H} |\chi^\Gamma(h)|^2 + \sum_{h\in H} \omega^{nk}|\chi^\Gamma(t^k h)|^2 + \ldots = \delta_{np}|G|\ .$$

If we sum the p relations and note that

$$\sum_{n=1}^{p} \omega^{kn} = p\ \delta_{kp}\ ,$$

we obtain

$$p \sum_{h\in H} |\chi^\Gamma(h)|^2 = |G| = p\ |H|\ .$$

This equation shows that Γ_H is an irrep of **H** and therefore $\langle\Gamma|\gamma\rangle = 1$.

Since by definition a solvable group always has a composition series such that its factor groups are cyclic subgroups of prime order we conclude that a composition series of a solvable group is always canonical.

III. LABELS

Let Γ be an irrep of the group $\mathbf{G}$ with conjugation classes C_i. If $|\Gamma|$ is the dimension of Γ, let us define an operator

$$\mathbf{P}^{\Gamma}(\mathbf{G}) = (|\Gamma|/|\mathbf{G}|) \sum_{g\in\mathbf{G}} \chi^{\Gamma}(g)^{*}g = (|\Gamma|/|\mathbf{G}|) \sum_{i} \chi^{\Gamma}(C_i)^{*}S(C_i), \quad (6)$$

where

$$\chi^{\Gamma}(g) = \sum_{k=1}^{|\Gamma|} \Gamma(g)_{kk} \quad \text{and} \quad S(C_i) = \sum_{g\in C_i} g$$

are the elements of the center of the algebra of $\mathbf{G}$.

From the orthogonality relations for the characters $\chi^{\Gamma}(g)$, it is easy to proof that

$$\mathbf{P}^{\Gamma}(\mathbf{G})\, \mathbf{P}^{\Gamma'}(\mathbf{G}) = \delta_{\Gamma\Gamma'}\, \mathbf{P}^{\Gamma}(\mathbf{G}).$$

Moreover, we must note that if $g^{-1}= g^{\dagger}$, $\mathbf{P}^{\Gamma}(\mathbf{G})$ is a self-adjoint operator and therefore, it is a projection operator.

On the other hand, if the elements of $\mathbf{G}$ are not unitary operators, $\mathbf{P}^{\Gamma}(\mathbf{G})$ is not a self-adjoint operator but if $\mathbf{G}$ is a finite group it is always possible to take $\Gamma(g)^{\dagger}= \Gamma(g^{-1})$, and in this case the representations of $\mathbf{P}^{\Gamma}$ in the bases of the irreps of $\mathbf{G}$ are self-adjoint matrices. Thus, our results are still valid.

Equation (6) can be inverted to give

$$S(C_i) = |\Gamma|^{-1} \sum_{\Gamma} \chi^{\Gamma}(C_i)\, \mathbf{P}^{\Gamma}(\mathbf{G}) . \quad (7)$$

This equation shows that the representations of the operators $S(C_i)$ within the space $|\Gamma\gamma\rangle$ are given by diagonal matrices with eigenvalues $\chi^{\Gamma}(C_i)/|\Gamma|$.

In order to construct the self-adjoint operator which labels the bases of the irreps of a finite group, we define the operator given by

$$N(G) = \sum_n n\, P^{\Gamma_n}(G) = \sum_i a_i\, S(C_i)\ ,$$

where $a_i = |G|^{-1} \sum_n n\, |\Gamma_n|\, \chi^{\Gamma_n}(C_i)^*$.

Then, we see that N(G) can be calculated using only a character table of the group **G**.

Now, if we have a sequence $G_0 \supset G_1 \supset \ldots \supset G_\ell$, and being b-1 an upper limit to the number of irreps of each subgroup G_i of the series, the labeling operator is defined by

$$A = \sum_{k=0}^{\ell} b^{\ell-k}\, N(G_k)\ .$$

Since the operators $N(G_k)$ commute $\forall$ k, the eigenvalues λ_j of **A** have the form $\lambda_j = n_0 n_1 \ldots n_\ell$, and are integer numbers in base b.

Let us take specifically the sequence

$$O_h^* \supset \ldots \supset G_k \times C_i \supset \ldots \supset G_\ell \times C_i,$$

where G_k are subgroups of O^* (e.g. Caride and Zanette 1985). We can define the corresponding labeling operator by

$$A = \sum_{k=0}^{\ell} 10^{\ell-k}\, N(G_k)\ i\ ,$$

where i is the inversion operator. This definition allows the direct determination of the parity of the basis through the sign of the eigenvalues. On the other hand, the irreps which are symmetry adapted to the given chain, are also adapted to sequences of the type

$$\mathbf{O}_h^* \supset \ldots \supset \mathbf{G}_k \times \mathbf{C}_i \supset \mathbf{G}_k' \supset \ldots \supset \mathbf{G}_\ell' \;,$$

where the $\mathbf{G}_k'$ are groups isomorphic to subgroups of $\mathbf{O}^*$. Since a subgroup of $\mathbf{O}_h^*$ is either a direct product of a subgroup of $\mathbf{O}^*$ and the inversion or it is isomorphic to a subgroup of $\mathbf{O}^*$ we only need eight sets of adapted irreps (e.g. Nogueira et al 1986) to represent all the sequences of $\mathbf{O}_h^*$, each set corresponding to one sequence of $\mathbf{O}^*$.

The calculation of the bases of the irreps of a group $\mathbf{G}$ performed as if they were eigenfunctions of invariant operators unables also the calculation of the Clebsch-Gordan coefficients. Here we show that the use of the eigenfunctions of the operator $\mathbf{A}$, drastically simplifies the calculation of the coefficients.

Let $|\lambda_3 n\rangle$ be an eigenfunction of $\mathbf{A}$ which appears as the result of the couppling of the functions $|\lambda_1\rangle|\lambda_2\rangle$, being n the label for the repeated representations λ_3 in the product space. Then,

$$|\lambda_3 n\rangle = \sum_{\lambda_1,\lambda_2} |\lambda_1\rangle|\lambda_2\rangle \langle\lambda_1\lambda_2|\lambda_3 n\rangle \;.$$

Applying the operator $\mathbf{A}$ on this equation and after a simple algebra we obtain

$$\Omega(\lambda_1\lambda_2,\lambda_1'\lambda_2') \langle\lambda_1'\lambda_2'|\lambda_3 n\rangle = \lambda_3 \langle\lambda_1\lambda_2|\lambda_3 n\rangle \quad ,$$

where

$$\Omega(\lambda_1\lambda_2\lambda_1'\lambda_2') = \sum_i a_i \left(\sum_{g\in C_i} \langle\lambda_1|g|\lambda_1'\rangle \langle\lambda_2|g|\lambda_2'\rangle \right).$$

Our choice of the bases forces the following condition on the matrix elements

$\langle\lambda|g|\lambda'\rangle \neq 0 \quad (\forall \quad g\in G)$ if and only if $|\lambda-\lambda'| < n^{\ell-k}$.

Clearly, if we take this condition into account when obtaining the Clebsch-Gordan coefficients, the number of matrix elements to be calculated is greatly reduced.

IV. RESULTS AND DISCUSSION

Let G be a group with a series

$$G_0 \supset G_1 \supset \ldots \supset G_\ell \quad ,$$

and let $|\lambda,\nu\rangle$ be the functions which are linear combinations of the basis vectors of a vector space V such that the action of the operator A defined in Section III is given by

$$A\ |\lambda,\nu\rangle = \lambda\ |\lambda,\nu\rangle \ ,$$

where ν numbers the linear combinations which have the same value of $\lambda = n_0 n_1 \ldots n_\ell$.

In order to obtain a solution for ν, let us calculate the matrix element of an operator $\hat{H}_i$ which is such that $[g,\hat{H}_i]_- = 0,\ \forall\ g\in G_i$

$$\langle\lambda,\nu|\hat{H}_i|1',\nu'\rangle = \langle n_0 n_1 \ldots n_\ell,\nu|\hat{H}_i|n_0' n_1' \ldots n_\ell',\nu'\rangle \prod_{k=i}^{\ell} \delta_{n_k n_k'}$$

From this equation we see that if the eigenvalues of the term $\hat{H}_0$ are all different within each subset $|\lambda,\nu\rangle$ for fixed λ, we can label uniquely the bases of G_0 which are symmetry adapted to the given sequence.

Kramer and Moshinsky (1966) have shown that this is the case of the invariant operator $\hat{T}$ of O_h^* obtained from the spherical harmonics Y_{4m} within the vector spaces $V_j=\{|jm\rangle\}$ for fixed j.

Now we are going to show that we can add to $\mathbf{A}$ operator another term such that we will have a new self-adjoint operator with real eigenvalues consisting in an integer part (which is the old eigenvalue λ of $\mathbf{A}$) and a non-integer part corresponding to the eigenvalue of the operator $\hat{T}$.

Following Fox et al (1977) we write

$$\hat{T} = ((3/7)(2J+1))^{1/2}\,\hat{T}_0 + 1/3\ , \qquad (8)$$

with $\hat{T}_0 = (112/3(2J-3)_5)^{1/2}\,(-3J^4 + J^2 + 5(J_1^2 + J_2^2 + J_3^2))$,

where the J_i (i=1,2,3) are the components of the angular momentum J and,

$$(A)_k = A\,(A+1)\,\ldots\,(A+k-1)\ .$$

Then we define the new operator by

$$\hat{U} = (\sum_{k=0}^{\ell} 10^{\ell-k}\, N(G_k) + \hat{T})\ i$$

where the G_k are subgroups of $\mathbf{O}$ or $\mathbf{O}^*$ and, from equation (8), the eigenvalues t of $\hat{T}$ are in the interval (0,5/6). Since $\hat{T}$ commutes with every element $g\epsilon G$ it also commutes with $\mathbf{A}$ and therefore, the eigenvalues of $\hat{U}$ are given by

$$u = \pm\,(n_0 n_1\,\ldots\,n_\ell + t),$$

where the sign + (-) denotes that the subspace is even (odd) under the inversion operation.

It is important to note that the eigenvalues of $\hat{U}$ solve the problem of clustering observed by Fox et al in the eigenvalue spectrum of the operator $\hat{T} = T_{4A1}$ for $j > 20$.

Clearly, the considerations about T_{4A1} can be extended to the operator T_{6A1} which has the same type of tridiagonal matrix representation in the same subspace. This allows us to conclude that the bases of the operators $A + \alpha T_{4A1}$ and $A + \alpha T_{4A1} + \beta T_{6A1}$ (α and β arbitrary constants) are the more convenient functions to study problems refering to localized d and f electrons.

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