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On the labelling and symmetry adaptation of the solvable finite group representations

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Abstract. We propose a method to simultaneously perform a symmetry adaptation and a labelling of the bases of the irreducible representations of the solvable finite groups. It is performed by defining a self-adjoint operator with eigenvalues which show the descent in symmetry of the irreps of the group-subgroup sequences. We also prove a theorem on the canonicity of the composition series of finite groups.

1. Introduction

Group theory is a powerful tool for the study of the physical properties of quantum mechanical systems. In order to exploit the symmetry properties of the systems effectively, 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 labelling of the bases of the irreducible representations (irreps) of the finite groups associated with physical problems.

In § 2 we show that a composition series of a solvable group is always a canonical sequence, an essential requirement for the labelling to be unique. This is a highly desired result since the majority of the groups associated with solid state physics and quantum chemistry problems are solvable groups—as is the case of crystallographic groups, point groups, Shubnikov groups, etc. We also show that the sequences of a finite group which has a derived series ending with a group isomorphic to an alternating group are canonical series.

The labelling of the basis functions of the head group in a sequence is performed in § 3, where we show that it is possible to construct a self-adjoint operator for each one of the sequences of the type $G_0 \supset G_1 \supset \ldots \supset G_l$, such that the eigenvalues show the descent in symmetry in the chain and the corresponding eigenvectors actually may be taken to be the symmetry adapted bases of the irreps.

The key to the labelling consists essentially of adopting the general Bethe 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 § 3 that, in order to construct the labelling operators, we only need a character table of the groups involved in the sequence and that the diagonalisation of a particular linear combination of the right and left regular representations of the labelling operator gives the irreps adapted to a canonical sequence.

The extension of the method to label the bases of vector fields is analysed in § 4 where we also propose a solution for the cubic harmonics, i.e. the labelling of the bases for the sequence $SU(2) \supset O^* \supset \ldots$.

2. Canonical sequences

First we recall that a group has a canonical sequence when the number of times each irrep of each subgroup in the sequence occurs in the restriction of the representation of the corresponding preceding group is either one or zero.

We must note that we are going to deal only with canonical sequences ending with Abelian groups, since this is the necessary and sufficient condition for the labelling to be unique.

Let a subclass of $g \in G$ be the set of elements $\{hgh^{-1} | h \in H\}$, where $H \subset G$. Wigner (1968) has shown that, if all the subclasses so defined commute, $G \supset H$ is a canonical sequence. The original application of Wigner's theorem was confined to the demonstration that the sequences of symmetric groups $S_n \supset S_{n-1} \supset \ldots \supset S_2$ are canonical sequences for all degrees n. We shall prove now that if H is an invariant subgroup of G such that $G/H \sim C_p$, i.e. a cyclic group of prime order, the sequence $G \rhd H$ is a canonical sequence and since all the factors of a composition series of a solvable group are isomorphic to cyclic groups of prime order, we shall conclude that a solvable group always has a composition series that is canonical. Furthermore, we shall show that it is possible to construct canonical series for groups which are not solvable but have derived series ending with a simple group isomorphic to an alternating group A_n of degree $n > 5$.

Let γ be an irrep of H, a proper maximal normal subgroup of G. The stabiliser of γ in G is given by

$$S_G(\gamma) = \{g \in G | \gamma^g(h) = \gamma(ghg^{-1}) \sim \gamma(h)\} \forall h \in H. \tag{1}$$

According to this,

$$H \subseteq S_G(\gamma) \subseteq G \tag{2}$$

and we can decompose G into cosets of $S_G(\gamma)$.

If $t_1, \ldots, t_l$ are the representatives of the cosets, with $t_1 = 1$ and $l = |G|/|S_G(\gamma)|$, H has l different conjugate irreps given by

$$\gamma_k(h) = \gamma(t_k h t_k^{-1}). \tag{3}$$

Since

$$\langle \Gamma | \gamma \rangle = (1/|H|) \sum_{h \in H} x^\Gamma(h) x^\gamma(h)^*$$

and

$$x^\Gamma(ghg^{-1}) = x^\Gamma(h)$$

we have

$$\langle \Gamma | \gamma_k \rangle = \langle \Gamma | \gamma \rangle \qquad \text{for } k = 1, \ldots, l. \tag{4}$$

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

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

$$x^{\gamma^G}(h) = \sum_{i=1}^{l} x^\gamma(t_i h t_i^{-1}) = \sum_{i=1}^{l} x^{\gamma_i}(h) \tag{5}$$

we conclude that the γ_i are the only irreps contained in Γ_H.

Then we can write

$$x^{\Gamma}(h)=\langle\Gamma|\gamma\rangle\sum_{i=1}^{l}x^{\gamma_i}(h) \tag{6}$$

and from the orthogonality of the characters we have

$$\begin{aligned}\sum_{\gamma}\langle\Gamma|\gamma\rangle^2&=\sum_{i=1}^{l}\langle\Gamma|\gamma_i\rangle^2\\&=\langle\Gamma|\gamma\rangle^2|G|/|S_G(\gamma)|\\&=(1/|H|)\sum_{h\in H}|x^{\Gamma}(h)|^2\leq|G|/|H|.\end{aligned} \tag{7}$$

It then follows that

$$\langle\Gamma|\gamma\rangle^2\leq|S_G(\gamma)|/|H|. \tag{8}$$

Now, if the invariant subgroup H of G is such that $|G/H|=p$ (a prime number), from equation (2) we have that either $S_G(\gamma)=H$ or $S_G(\gamma)=G$.

In the first case, equation (8) yields $\langle\Gamma|\gamma\rangle=1$ and consequently

$$\Gamma(h)=\sum_{i=1}^{p}\gamma_i(h). \tag{9}$$

Therefore, $x^{\Gamma}(g)=0\ \forall g\in\{G-H\}$ is a necessary condition for $S_G(\gamma)=H$. But it is also a sufficient condition, because if $S_G(\gamma)=G$, there would be at least one conjugation class C of G contained in $\{G-H\}$ such that $x^{\Gamma}(C)\neq 0$. But if $x^{\Gamma}(g)=0\ \forall g\in\{G-H\}$, the equality holds in equation (8) and therefore $\langle\Gamma|\gamma\rangle^2=p$ in contradiction with our assumption that p is a prime number.

In the second case, i.e. $S_G(\gamma)=G$, as $G/H\sim C_p$, there are in G at least p one-dimensional representations λ_n of the form $\lambda_n(t^kH)=\omega^{nk}$, 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 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

$$\begin{aligned}\Gamma_n(t^kh)&=\lambda_n(t^kH)\Gamma_p(t^kh)\\&=\omega^{nk}\Gamma_p(t^kh)\qquad\forall h\in H, 0<n<p\quad\text{and}\quad\Gamma_p\equiv\Gamma.\end{aligned} \tag{10}$$

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

$$\sum_{h\in H}|x^{\Gamma}(h)|^2+\sum_{h\in H}\omega^{nk}|x^{\Gamma}(t^kh)|^2+\ldots=\delta_{np}|G|. \tag{11}$$

If we sum the p relations and note that

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

we obtain

$$p\sum_{h\in H}|x^{\Gamma}(h)|^2=|G|=p|H|. \tag{12}$$

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

Since 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.

Let us suppose now that G is not solvable. In this case it has a derived series $G \triangleright G' \triangleright G'' \triangleright \ldots$ which ends with a non-Abelian simple group different from unity. If the tail group is isomorphic to a group A_n it is still possible to construct a canonical sequence for G. This can be simply done by refining the derived series (Kurosh 1960) until all the factor groups are simple Abelian groups. Next, the series can continue with the canonical sequence $A_n \supset A_{n-1} \supset \ldots \supset A_3$ (Luan Dehuai and Wybourne 1981). On the other hand it can happen that, if $G_l = A_n$, G_{l-1} could be S_n (since $S_n' = A_n$). In this case, it is also possible to construct the alternative canonical sequence

$$G \triangleright G' \triangleright \ldots \triangleright G_{l-1} \supset S_{n-1} \supset \ldots \supset S_2.$$

It is interesting to note that if H is not a normal subgroup of G, the sequence $G \supset H$ is still a canonical series if the index of H in G satisfies $|G:H| \leqslant 3$ or $|G:H| = 4$ in the special case when

$$H_G^{\text{core}} = \bigcap_{g \in G} gHg^{-1} \subseteq Z(G)$$

where Z(G) is the group of the centre of G (Caride *et al* 1987).

These general results on canonical sequences can be deduced for the crystallographic point groups by examination of branching rule tables, like those given by Butler (1981).

3. Labels and symmetry adapted irreps

Let G be a finite group with at least one canonical sequence $G_0 \supset G_1 \supset \ldots \supset G_i \supset \ldots$ ending with an Abelian group.

The aim of the present section is to construct a self-adjoint operator Λ as a linear combination of the principal idempotents in the algebra of the subgroups G_i (Klein *et al* 1970). This operator will allow us to adapt in symmetry the bases of a finite vector space such that the eigenvalues show the descent in symmetry of the irreps of the subgroups in the sequence. Due to the direct relation between principal idempotents and class sum operators (see equation (13) below), the operator Λ can be considered as a particular realisation of a complete set of commuting operators (CSCO I) defined by Chen *et al* (1985).

If we call ${}^{R}\Lambda$ and ${}^{L}\Lambda$ the right and left regular representations of the operator Λ, we shall show that a linear combination of ${}^{R}\Lambda$ and ${}^{L}\Lambda^*$ (* stands for complex conjugation) will give, by diagonalisation, the irreps of G which are symmetry adapted to the canonical sequence.

Let Γ be an irrep of a group G_k with conjugation classes C_i. If $|\Gamma|$ is the dimension of Γ, let us define an operator which is the expression of the principal idempotents of the algebra of G_k

$$\boldsymbol{P}^{\Gamma}(G_k) = (|\Gamma|/|G_k|) \sum_{g \in G_k} x^{\Gamma}(g)^* g = (|\Gamma|/|G_k|) \sum_i x^{\Gamma}(C_i)^* S(C_i) \qquad (13)$$

where

$$x^{\Gamma}(g) = \sum_{k=1}^{|\Gamma|} \Gamma(g)_{kk} \qquad S(C_i) = \sum_{g \in C_i} g$$

are the elements of the centre of the algebra of G_k.

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

$$\boldsymbol{P}^{\Gamma}(G_k)\boldsymbol{P}^{\Gamma'}(G_k) = \delta_{\Gamma\Gamma'} \boldsymbol{P}^{\Gamma}(G_k).$$

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

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

Equation (13) can be inverted to give

$$S(C_i)=\sum_{\Gamma}|\Gamma|^{-1}x^{\Gamma}(C_i)\boldsymbol{P}^{\Gamma}(\mathrm{G}_k). \tag{14}$$

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 $x^{\Gamma}(C_i)/|\Gamma|$.

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

$$\boldsymbol{N}(\mathrm{G}_k)=\sum_{n} n\boldsymbol{P}^{\Gamma_n}(\mathrm{G}_k)=\sum_{i} a_i S(C_i) \tag{15}$$

where

$$a_i=|\mathrm{G}_k|^{-1}\sum_{n} n|\Gamma_n|x^{\Gamma_n}(C_i)^{*}.$$

Then we see that $\boldsymbol{N}(\mathrm{G}_k)$ can be calculated using only the character table of the group G_k.

Now, if we have a sequence $\mathrm{G}_0\supset\mathrm{G}_1\supset\ldots\supset\mathrm{G}_l$, and $b-1$ is an upper limit to the number of irreps of each subgroup G_i of the series, the labelling operator is defined by

$$\Lambda=\sum_{k=0}^{l} b^{l-k}\boldsymbol{N}(\mathrm{G}_k). \tag{16}$$

Since the operators $\boldsymbol{N}(\mathrm{G}_k)$ commute $\forall k$, the eigenvalues λ_j of Λ have the form $\lambda_j=n_0n_1\ldots n_l$, and are integer numbers in base b.

As an example of the utilisation of Λ let us take the canonical sequence $\mathrm{C}_{4\mathrm{v}}\supset\mathrm{C}_2(\sigma^{yz})$. From a table of characters of these groups we can write our labelling operator in the following form:

$$\Lambda=b\boldsymbol{N}(\mathrm{C}_{4\mathrm{v}})+\boldsymbol{N}(\mathrm{C}_2)$$

where

$$\boldsymbol{N}(\mathrm{C}_{4\mathrm{v}})=\tfrac{1}{4}[20e-(5e+2C_4^z+\sigma^{yz})(e+C_2^z)]$$

$$\boldsymbol{N}(\mathrm{C}_2)=\tfrac{1}{2}(3e-\sigma^{yz}).$$

When we apply Λ to the irreducible space (xyz), and $b>5$, we obtain the diagonal matrix

$$(\Lambda)=\begin{pmatrix}52 & & \\ & 51 & \\ & & 11\end{pmatrix}.$$

Therefore, the corresponding bases for the irreps Γ_i, Γ_j of $\mathrm{C}_{4\mathrm{v}}\supset\mathrm{C}_2$ are

$$|\Gamma_5\Gamma_2\rangle=x \qquad |\Gamma_5\Gamma_1\rangle=y \qquad |\Gamma_1\Gamma_1\rangle=z.$$

We shall now show how we can use the operator Λ to calculate the symmetry adapted irreps corresponding to a canonical sequence. For this purpose, let us call $\Gamma(g)_{\lambda\lambda'}$ the matrix elements of a symmetry adapted irrep of G to the canonical sequence $G=G_0 \supset \ldots \supset G_l$, bearing in mind that G_l is Abelian.

In order to simplify the notation, we omit the subindex n_0 in Γ, since $\Gamma(g)_{\lambda\lambda'} \neq 0$ if and only if

$$\lambda = n_0 n_1 \ldots n_l \qquad \lambda' = n_0 n'_1 \ldots n'_l .$$

Further, as $\Gamma(g)$ is supposed to be symmetry adapted to the sequence, we must have

$$\Gamma(g)_{\lambda\lambda'} = \left(\prod_{k=0}^{i} \delta_{n_k, n'_k}\right)\Gamma(g)_{\mu\mu'} \qquad \forall g \in G_i \tag{17}$$

for i within the interval $(0, l)$ and where

$$\mu = n_i n_{i+1} \ldots n_l \qquad \mu' = n_i n'_{i+1} \ldots n'_l .$$

From the definition of Λ, the ijth matrix element of its left regular representation is given by

$${}^{\mathrm{L}}\Lambda_{ij} = \sum_k b^{l-k} \sum_{n_k} \{n_k |x^{n_k}(1)|/|G_k|\} \sum_{g \in G_k} x^{n_k}(g)^* \delta_{g_i, gg_j} . \tag{18}$$

From equations (17) and (18) and the orthogonality of the irreps of a finite group, we have

$$\sum_j {}^{\mathrm{L}}\Lambda_{ij}\Gamma(g_j)^*_{\lambda\lambda'} = \lambda\Gamma(g_i)^*_{\lambda\lambda'} \tag{19}$$

which shows that the element $\Gamma(g_j)^*_{\lambda\lambda'}$ $(j=1, \ldots, |G|)$ is the jth component of the eigenvector of the left regular representation of Λ.

If we now write the matrix elements of the right regular representation, we have

$${}^{\mathrm{R}}\Lambda_{ij} = \sum_k b^{l-k} \sum_{n_k} \{n_k |x^{n_k}(1)|/|G_k|\} \sum_{g \in G_k} x^{n_k}(g)^* \delta_{g_i, g_j g^{-1}} \tag{20}$$

which applied to the elements of $\Gamma(g_j)$ results in

$$\sum_j {}^{\mathrm{R}}\Lambda_{ij}\Gamma(g_j)_{\lambda\lambda} = \lambda'\Gamma(g_i)_{\lambda\lambda'} . \tag{21}$$

Therefore, from equations (19) and (21) and taking into account that ${}^{\mathrm{L}}\Lambda$ and ${}^{\mathrm{R}}\Lambda$ commute, we have that the normalised eigenvectors of the matrix

$$\boldsymbol{Y} = {}^{\mathrm{L}}\Lambda^* b^l + {}^{\mathrm{R}}\Lambda \tag{22}$$

are given, up to a phase factor, by

$$y^{\beta}(g_i) = (|\Gamma|/|G|)^{1/2}\Gamma(g_i)_{\lambda\lambda'} \tag{23}$$

where the eigenvalue β is an integer number of the form

$$\beta = \lambda\lambda' = n_0 n_1 \ldots n_l n_0 n'_1 \ldots n'_l .$$

Our $\boldsymbol{Y}$ matrix can also be interpreted as a realisation of a particular linear combination of the CSCO II of Chen *et al.* The advantage of $\boldsymbol{Y}$ is obvious if we want to calculate the symmetry adapted irreps corresponding to a canonical series. Furthermore, it avoids the introduction of the intrinsic group, anti-isomorphic to G, generated by a right shift. Instead, we have the right regular representation which is isomorphic to G.

Let us calculate as an example the eigenvectors and eigenvalues of the operator $\boldsymbol{Y}$ corresponding to the sequence $C_{4v} \supset C_2(\sigma^{yz})$.

Since the characters of the irreps of both groups are real numbers, we only need to calculate the left regular representation of Λ and add the right regular representation multiplied by b^2. The unitary matrix that diagonalises the representation of $\boldsymbol{Y}$ is

$$\boldsymbol{M} = (2\sqrt{2})^{-1} \begin{pmatrix} 1 & 1 & 1 & 1 & \sqrt{2} & 0 & 0 & \sqrt{2} \\ 1 & 1 & -1 & -1 & 0 & -\sqrt{2} & \sqrt{2} & 0 \\ 1 & 1 & 1 & 1 & -\sqrt{2} & 0 & 0 & -\sqrt{2} \\ 1 & 1 & -1 & -1 & 0 & \sqrt{2} & -\sqrt{2} & 0 \\ 1 & -1 & -1 & 1 & \sqrt{2} & 0 & 0 & -\sqrt{2} \\ 1 & -1 & 1 & -1 & 0 & -\sqrt{2} & -\sqrt{2} & 0 \\ 1 & -1 & -1 & 1 & -\sqrt{2} & 0 & 0 & \sqrt{2} \\ 1 & -1 & 1 & -1 & 0 & \sqrt{2} & \sqrt{2} & 0 \end{pmatrix}$$

where each column corresponds to the eigenvalues 1111, 2222, 3232, 4141, 5151, 5152, 5151 and 5252, respectively.

4. Results and discussion

Let G be a group with a series

$$G_0 \supset G_1 \supset \ldots \supset G_l$$

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 Λ defined in § 3 is given by

$$\Lambda|\lambda, \nu\rangle = \lambda|\lambda, \nu\rangle \tag{24}$$

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

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

$$\langle\lambda, \nu|\hat{\boldsymbol{H}}_i|l', \nu'\rangle = \langle n_0 n_1 \ldots n_l, \nu|\hat{\boldsymbol{H}}_i|n'_0 n'_1 \ldots n'_l, \nu'\rangle \prod_{k=i}^{l} \delta_{n_k n'_k}.$$

From this equation we see that, if the eigenvalues of the term $\hat{\boldsymbol{H}}_0$ 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 $\hat{\boldsymbol{T}}$ of O_h^* obtained from the spherical harmonics Y_{4m} within the vector spaces $V_j = \{|jm\rangle\}$ for fixed j.

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

Following Fox *et al* (1977) we write

$$\hat{\boldsymbol{T}} = [\tfrac{3}{7}(2J+1)]^{1/2}\hat{T}_0 + \tfrac{1}{3} \tag{25}$$

with

$$\hat{T}_0 = [112/3(2J-3)_9]^{1/2}[-3\boldsymbol{J}^4 + \boldsymbol{J}^2 + 5(\boldsymbol{J}_1^2 + \boldsymbol{J}_2^2 + \boldsymbol{J}_3^2)]$$

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

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

Then we define the new operator by

$$\hat{U} = \left(\sum_{k=0}^{l} 10^{l-k} N(\mathrm{G}_k) + \hat{T}\right) i \tag{26}$$

where the G_k are subgroups of O or O*, i is the inversion operator and, from equation (25), the eigenvalues t of $\hat{T}$ are in the interval $(0, \frac{5}{6})$. Since $\hat{T}$ commutes with every element $g \in \mathrm{G}$ it also commutes with Λ and, therefore, the eigenvalues of $\hat{U}$ are given by

$$u = \pm(n_0 n_1 \dots n_l + t) \tag{27}$$

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 $\Lambda + \alpha T_{4A1}$ and $\Lambda + \alpha T_{4A1} + \beta T_{6A1}$ (α and β arbitrary constants) are more convenient functions to study problems referring to localised d and f electrons.

Finally, we want to point out some considerations on finite groups with canonical series.

(i) Apart from A_5 and A_6, there exist among the groups of order less than 1000 only three simple groups (Suzuki 1982), of which it is not known if they have canonical sequences.

(ii) Any group of odd order is solvable (Suzuki 1986).

(iii) The class of solvable groups is closed with respect to the formation of subgroups, images and extensions of its members (Robinson 1982).

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