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Continuous group invariances of linear Jahn–Teller systems in icosahedral symmetry: extension to direct sum electronic spaces

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Abstract. Previous results for the generation of linear, icosahedral, Jahn–Teller (JT) Hamiltonians with continuous group symmetries are extended. It is demonstrated that it is possible to define electronic generalized tensor operators on a direct sum electronic space such that a set of these operators is closed under commutation with another set of electronic generalized tensor operators which act as the generators of a continuous group. The normal modes carrying irreducible representations of the continuous group are then coupled 'equally' to produce a JT Hamiltonian which is invariant under the operations of the continuous group. The continuous groups generated on the direct sum spaces $(T_1 \oplus T_2)$, $(T_i \oplus G)$, $(T_i \oplus H)$ and $(G \oplus H)$ are discussed in detail. These additional continuous groups are of interest when the lowest JT states of certain icosahedral JT systems (such as some of those found in C_{60}) are modelled. The additional continuous group symmetry allows an analytic diagonalization of the linear JT matrix to be provided and thus facilitates an exact treatment of the vibronic ground state for these models.

1. Introduction

In neutral C_{60}, a molecule with icosahedral symmetry, the highest occupied molecular orbital (HOMO) is found to be a filled orbital of h_u symmetry [4]. The lowest unoccupied molecular orbital (LUMO) is found to be of t_{1u} type. Exciting an electron from the HOMO into the LUMO produces an excitation which may then have the symmetry characteristics of any of the irreducible representations (irreps) found in the decomposition of the direct product of these two irreps, $h_u \otimes t_{1u} = T_{1g} \oplus T_{2g} \oplus G_g \oplus H_g$. The presence of such excitations will cause the icosahedral molecule to suffer a Jahn–Teller (JT) interaction even though in its ground state the neutral molecule does not. Negri *et al* [8] make some numerical predictions as to the ordering of the lowest exciton states in C_{60} as do Lazlo and Udvardi [7]. It is clear from the results of these two studies that the behaviour of closely spaced exciton states of T_1, T_2, G and H symmetry will be of interest. The work in this paper was motivated by the search for ways in which JT systems of, for example, the type $(T_{1g} \oplus T_{2g}) \otimes (h \oplus g)$ could be treated analytically. Such a type of JT system could be found in the lowest exciton states of neutral C_{60}.

In studying strong JT coupling problems, one problem in the analysis is to analytically diagonalize the linear JT matrix associated with the problem. If this is possible then the JT electronic ground state, the lowest energy eigenvector of the JT matrix, is immediately

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known and the form of the Born–Oppenheimer vibronic ground state may be determined. In many other JT systems that have previously been considered, for example $T \otimes h$ and $G \otimes (g \oplus h)$ [2] in icosahedral symmetry, an exact analytical treatment in strong coupling has been possible due to the presence of unexpectedly high symmetry (above that of the point group for the molecular system) in the linear JT Hamiltonian of the problem. This unexpected continuous group symmetry, which in the above cases is SO(3) and SO(4) respectively, allowed orthogonal transformations to be determined which diagonalize the associated JT matrix. In initiating this body of work it was hoped that it would be possible to find further continuous group symmetries associated with the linear JT Hamiltonians for problems of the type $(\Gamma_i \oplus \Gamma_j) \otimes \Sigma\lambda$ that may occur in the neutral C_{60} exciton spectrum.

In a paper in 1980 [11], Pooler provided a method for generating linear JT Hamiltonians with continuous group symmetries that is applicable to all real character simple phase groups. This was an extension from earlier work [9] which had itself generalized the theory of the generation of continuous groups of irreducible electronic operators for the rotation group [6], to include simply reducible groups and the cubic double group.

The method that Pooler demonstrated involved defining a set of odd and even [9] electronic generalized tensor operators on a single irreducible electronic space. (In his definition even operators are those which always occur in the symmetric part of the direct product of an integer representation with itself, while those which occur in the antisymmetric part are defined as odd). The odd operators were shown to be closed under commutation amongst themselves, so forming the generators of a continuous group. Under the action of commutation with these generators, the even operators were transformed amongst themselves, and hence were seen to carry irreps of the continuous group. It was shown that if the even electronic operators are coupled to suitably chosen vibrational coordinates, a linear JT Hamiltonian that is a scalar under the operations of the group may be formed, provided that the coupling strengths of the modes associated with a particular irrep, carried by the even operators, are in the same ratio as certain isoscalars (section 3).

In this paper it is shown that it is possible to define electronic generalized tensor operators on an electronic space that is a direct sum of more than one irreducible space, with the odd operators again forming the generators of a continuous group, and another set of operators carrying irreps of that group. It is precisely this result that was sought in order to allow an analytic treatment of $(\Gamma_i \oplus \Gamma_j) \otimes \Sigma\lambda$ JT problems.

In section 2 the notation to be employed in this paper is introduced and some of the relevant group theory is discussed briefly. In section 3 a concise account of Pooler's results for the generation of continuous groups using operators defined on a single irreducible electronic space is provided, and 'equal' coupling is defined. In section 4 it is demonstrated that the Judd–Pooler method may be extended, allowing the generators of a continuous group to be defined on a space that is the direct sum of irreducible electronic spaces. The tensorial notation of Derome and Sharp [3], as elucidated by Butler [1], is used, as general relations for the commutation of 'direct sum' tensor operators are obtained. The specific implications for irreps of the icosahedral group are presented. In section 5 the continuous groups that may be generated on the icosahedral electronic spaces $(T_1 \oplus T_2)$, $(T_i \oplus G)$, $(T_i \oplus H)$ and $(G \oplus H)$ are examined in detail and the form of the invariant linear JT Hamiltonians are provided. In the appendix, section A.1 contains a derivation of the way in which it is possible to define generalized tensor operators on a direct sum space and section A.2 provides a derivation of the way in which a product of two such generalized tensor operators may be expressed as a linear sum of other such generalized tensor operators.

Although the results in sections A.1 and A.2 are not new, their application in this paper is novel and this work is included for completeness. The sections A.3–A.5 contain tables listing the way in which icosahedral operators are embedded in the operators that transform as irreps of the continuous groups.

2. Notation and definitions

In this paper the manipulation of symmetrized coupling coefficients will figure in many of the calculations. It will prove convenient to make use of both the tensorial notation of Derome and Sharp [3], as well as the generalized [1] Wigner notation. The tensorial notation provides clarity when raising and lowering indices on complex conjugation and for that reason it is used in the derivation of the general results of section 4 and in the appendix. The icosahedral basis used by Pooler in deriving his tables of 3-jm and 6-j symbols [10] is employed in sections 3 and 5, and here the generalized Wigner notation is used in accordance with the original papers by Pooler. All the applications in this paper will deal with the icosahedral group which is an example of a real character simple phase group. A real character group is one in which the representation complex conjugate to λ is equivalent to λ: $\lambda = \lambda^*$. A simple phase group is one in which the 3-jm symbols may be defined such that permutation of their columns results only in a phase change.

In the generalized Wigner notation, the 3-jm symbol is represented by

$$\begin{pmatrix} \Lambda_1 & \Lambda_2 & \Lambda_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}^r \tag{1}$$

where the γ's label the irrep basis and r is a multiplicity label distinguishing between repeated irreps in $\Lambda_1 \otimes \Lambda_2 = \Sigma \Lambda_3$. In the tensorial notation the 3-jm symbol is equivalently defined as

$$(\Lambda_1 \Lambda_2 \Lambda_3)_{r\gamma_1\gamma_2\gamma_3}. \tag{2}$$

A unitary matrix, the 1-jm symbol, $(\lambda)_{ij}$, which connects irreps, $\lambda(R)$, with their complex conjugates, $\lambda^*(R)$, may be defined. This symbol also allows a raising operation to be defined [1]

$$(\lambda)^{i_1 j_1} (\lambda_1^* \lambda_2 \lambda_3)_{r j_1 i_2 i_3} = (\lambda_1 \lambda_2 \lambda_3)_r{}^{i_1}{}_{i_2 i_3} \tag{3}$$

where the summation over repeated indices is implicit, as will be the case in all the use of the tensor notation, unless specifically indicated otherwise. Pooler provides an explicit form for the 1-jm symbol for the icosahedral group,

$$(\lambda)_{ij} = |\lambda|^{\frac{1}{2}} (\lambda\lambda A)_{1ij0} = \delta(i, -j) \tag{4}$$

where A is the identity irrep and $|\lambda|$ is the dimensionality of the irrep λ. It should be noted that when $\lambda = A$, i and j are both zero and $|\lambda| = 1$ so that $(A)_{00} = 1$ as required.

Coupled tensors may be defined by

$$\{P^{\lambda_1} Q^{\lambda_2}\}_i^{r\lambda} = |\lambda|^{\frac{1}{2}} \phi_\lambda (\lambda_1 \lambda_2 \lambda)^{r i_1 i_2}{}_i P_{i_1}^{\lambda_1} Q_{i_2}^{\lambda_2} \tag{5}$$

where ϕ_λ is the phase of the 1-jm symbol which may be taken to be $+1$ for all λ in the icosahedral group.

Another operation that will be of interest is that of permuting the columns of the 3-jm symbols. For simple phase groups phases may be chosen so that the 3-jm symbols are invariant under even column permutations and are multiplied by $\theta(\lambda_1\lambda_2\lambda_3 r) = \pm 1$ under odd ones. For the icosahedral group Pooler provides the result

$$\theta(\lambda_1\lambda_2\lambda_3 r) = (-1)^{\lambda_1+\lambda_2+\lambda_3}(-1)^{q(\lambda_1\lambda_2\lambda_3 r)} \tag{6}$$

where $q(\lambda_1\lambda_2\lambda_3 r)$ equals -1 if $(\lambda_1\lambda_2\lambda_3 r)$ is any permutation of $(HHG1)$ and $+1$ otherwise, and $(-1)^\lambda$ is given by

$$(-1)^\lambda = \begin{cases} +1 & \text{for } \lambda = A,\ G \text{ or } H \\ -1 & \text{for } \lambda = T_1 \text{ or } T_2. \end{cases} \tag{7}$$

6-j symbols will also appear in many of the manipulations in this paper and may be defined [1] as

$$\begin{Bmatrix} \lambda_1\lambda_2\lambda_3 \\ \mu_1\mu_2\mu_3 \end{Bmatrix}_{r_1r_2r_3r_4} = (\lambda_1\mu_2\mu_3)_{r_1 i_1}{}^{j_2}{}_{j_3}(\mu_1\lambda_2\mu_3)_{r_2 j_1 i_2}{}^{j_3}(\mu_1\mu_2\lambda_3)_{r_3}{}^{j_1}{}_{j_2 i_3}(\lambda_1\lambda_2\lambda_3)_{r_4}{}^{i_1 i_2 i_3}. \tag{8}$$

3. Electronic operators defined on a single irreducible electronic space

In [11], using electronic operators transforming as the irreps of a real character simple phase group, G, Pooler provides a method for generating linear JT Hamiltonians which exhibit continuous group symmetries.

In Pooler's notation electronic operators, $V_t^{r\Lambda}$, transforming as basis functions of the irrep Λ may be defined on an electronic basis $|\Gamma\gamma\rangle$ (which transforms as the irrep Γ under the operations of the real character simple phase group) as follows:

$$V_t^{r\Lambda} = \sum_{\gamma\gamma'} |\Lambda|^{\frac{1}{2}} \begin{pmatrix} \gamma & \Lambda & \Gamma \\ \Gamma & t & \gamma' \end{pmatrix}^r |\Gamma\gamma\rangle\langle\Gamma\gamma'|. \tag{9}$$

Pooler provides the commutation relation for operators of this type,

$$\begin{aligned}[V_\gamma^{r\Lambda}, V_{\gamma'}^{r'\Lambda'}] = \sum_{sr''\Lambda''\gamma''} & \begin{pmatrix} \Lambda & \Lambda' & \gamma'' \\ \gamma & \gamma' & \Lambda'' \end{pmatrix}^s \begin{Bmatrix} \Lambda & \Lambda' & \Lambda'' \\ \Gamma & \Gamma & \Gamma \end{Bmatrix}_{rr'r''s} (|\Lambda||\Lambda'||\Lambda''|)^{\frac{1}{2}} \\ & \times[\theta(\Gamma\Gamma\Lambda r)\theta(\Gamma\Gamma\Lambda' r') - \phi_\Gamma\theta(\Gamma\Gamma\Lambda'' r'')]V_{\gamma''}^{r''\Lambda''}. \end{aligned} \tag{10}$$

Using this relation and the expressions for θ and ϕ_Γ it is clear that odd operators commute amongst themselves and that the commutator of an odd operator and an even operator is a linear combination of even ones. Hence, the odd operators act as the generators of some continuous group, $\tilde{G}$, with the even operators carrying irreps of that group. Pooler uses the notation $M_t^{r\Lambda}$ for odd operators and $J_t^{r\Lambda}$ for even ones. Putting the generators of $\tilde{G}$ into standard form the transformation properties of the operators $V_t^{r\Lambda}$ may be obtained from their commutation relations with the generators. Hence, even operators carrying irreps of $\tilde{G}$ may be obtained and may be expressed as $J_{\tilde{\gamma}}^{\tilde{r}\tilde{\Lambda}}$.

Using these sets of operators which transform as irreps of G and $\tilde{G}$, Pooler considers two linear JT Hamiltonians, one invariant under G and one that is invariant under $\tilde{G}$, written respectively using (5) as

$$\begin{aligned} H_{JT}^{G} &= \sum_{r\Lambda} k_{r\Lambda}\{J^{r\Lambda}Q^{r\Lambda}\}_0^A|\Lambda|^{\frac{1}{2}} \\ H_{JT}^{\tilde{G}} &= \sum_{\tilde{r}\tilde{\Lambda}} \tilde{k}_{\tilde{r}\tilde{\Lambda}}\{J^{\tilde{r}\tilde{\Lambda}}Q^{\tilde{r}\tilde{\Lambda}}\}_0^{\tilde{A}}|\tilde{\Lambda}|^{\frac{1}{2}} \end{aligned} \tag{11}$$

where the $Q^{r\Lambda}$ and $Q^{\tilde{r}\tilde{\Lambda}}$ are sets of vibrational coordinates transforming in the same way as their respective electronic operators. A and $\tilde{A}$ are the identity irreps of their respective groups and k and $\tilde{k}$ are JT coupling constants. Here the group G is the symmetry group of the molecule with which the linear JT Hamiltonian H^{G}_{JT} is associated. Simultaneous transformation of the electronic operators and the vibrational coordinates under the group operations G in H^G and $\tilde{G}$ in $H^{\tilde{G}}$, leaves each Hamiltonian invariant. Clearly the Hamiltonian H^{G}_{JT} must be invariant under the symmetry group of the molecule. That it is possible to define another JT Hamiltonian $H^{\tilde{G}}_{JT}$ using a set of electronic and vibrational operators $J^{\tilde{r}\tilde{\Lambda}}$, $Q^{\tilde{r}\tilde{\Lambda}}$, which are linear combinations of the operators $J^{r\Lambda}$, $Q^{r\Lambda}$ of the group G and which transform as irreps of the group $\tilde{G}$ is at first sight merely an interesting peculiarity. However, using Racah's factorization lemma Pooler provides the result

$$H^{\tilde{G}}_{JT} = \sum_{r\tilde{r}\Lambda\tilde{\Lambda}} \tilde{k}_{\tilde{r}\tilde{\Lambda}} |\tilde{\Lambda}|^{\frac{1}{2}} \langle \tilde{r}\tilde{\Lambda} r\Lambda; \tilde{r}\tilde{\Lambda} r\Lambda || \tilde{A} A\rangle \{J^{r\Lambda} Q^{r\Lambda}\}^{A}_{0} \tag{12}$$

where the factor $\langle\, || \,\rangle$ is an isoscalar. This demonstrates that the Hamiltonian which is invariant under the group G is also invariant under the group $\tilde{G}$ if the coupling constants are related by factors depending upon certain isoscalars. 'Equal' coupling refers to the values of $k_{r\Lambda}$ and $\tilde{k}_{\tilde{r}\tilde{\Lambda}}$ that ensure the equality of these two Hamiltonians.

4. Electronic operators defined on an electronic space which is a direct sum of more than one irreducible space

In this section the properties of generalized tensor operators defined on a basis that is a direct sum of irreducible bases are discussed. Following Butler [1], a brief account of the general transformation properties of tensor operators, so defined, is presented. The commutation relations of direct sum tensor operators are then provided and the implications for the icosahedral group discussed.

4.1. General relations for the tensor operators of a real character simple phase group

Under the action of a group G the basis ket $|x\lambda i\rangle$ transforms as

$$O_R|x\lambda i\rangle = \sum_{i} |x\lambda j\rangle \lambda(R)_{ji} \tag{13}$$

where x enumerates distinct irreducible spaces with the same transformation properties given by the representation label λ, and i labels the basis within an irreducible space. A basis for linear operators may then be chosen to be

$$|x_1\lambda_1 i_1\rangle\langle x_2\lambda_2 i_2|. \tag{14}$$

Linear combinations of these operators may be formed such that linear operators transforming as irreps of the group are obtained. Such a combination may be expressed as

$$(r\lambda i(x_1\lambda_1, x_2\lambda_2)) = |\lambda|^{\frac{1}{2}} (\lambda_1\lambda\lambda_2)_{r}{}^{i_1}{}_{ii_2} |x_1\lambda_1 i_1\rangle\langle x_2\lambda_2 i_2| \tag{15}$$

and under the action of the group it may be shown (section A1) that this operator transforms as

$$O_R(r\lambda i(x_1\lambda_1, x_2\lambda_2))O_{R^{-1}} = (r\lambda j(x_1\lambda_1, x_2\lambda_2))\lambda(R)_{ji}. \tag{16}$$

This is (15.4) of [1]. This result demonstrates that a linear tensor operator may be defined on a basis transforming as $\lambda_1 \otimes \lambda_2^*$, where $\lambda_1 \neq \lambda_2$ in general.

Commutation relations for these tensor operators will now be derived. Consider the product of two such tensor operators,

$$
\begin{aligned}
&(r\lambda i(x_1\lambda_1, x_2\lambda_2))(r'\lambda' i'(x_1'\lambda_1', x_2'\lambda_2')) \\
&\qquad = (|\lambda||\lambda'|)^{\frac{1}{2}} (\lambda_1\lambda\lambda_2)_r{}^{i_1}{}_{ii_2} (\lambda_2\lambda'\lambda_2')_{r'}{}^{i_2}{}_{i'i_2'} |x_1\lambda_1 i_1\rangle\langle x_2'\lambda_2' i_2'| \delta_{x_2x_1'}\delta_{\lambda_2\lambda_1'}.
\end{aligned}
\tag{17}
$$

In A.2 it is demonstrated that for a real character simple phase group this product may be re-expressed as a sum over tensor operators defined on the product space $\lambda_1 \otimes \lambda_2'$, so that the right-hand side of (17) becomes

$$
\begin{aligned}
&= \sum_{\lambda_3} (|\lambda||\lambda'||\lambda_3|)^{\frac{1}{2}} (\lambda\lambda'\lambda_3)_{r_4 ii'}{}^{j} \begin{Bmatrix} \lambda & \lambda' & \lambda_3 \\ \lambda_2' & \lambda_1 & \lambda_2 \end{Bmatrix}_{rr'r_3r_4} \\
&\quad \times \theta(\lambda_1\lambda\lambda_2 r)\theta(\lambda_2\lambda'\lambda_2' r')(r_3\lambda_3 j(x_1\lambda_1, x_2'\lambda_2'))\delta_{x_2x_1'}\delta_{\lambda_2\lambda_1'}.
\end{aligned}
\tag{18}
$$

4.2. Commutation relations for tensor operators of the icosahedral group

From the discussion of Pooler's method in section 3 it is apparent that the behaviour under commutation of the electronic tensor operators associated with a JT problem will be of interest. When considering tensor operators defined on a single irreducible electronic space, odd operators were seen to be closed under commutation whilst the commutator of an odd and even operator produced a linear combination of the even operators. Consider table 1. Odd irreps within a Kronecker product are encased in $\{\}_A$ brackets. For even operators that are defined on the same irreducible space as a set of odd operators, the results of Pooler remain, with the odd operators generating a continuous group, irreps of which the even operators carry. Now, however, consider the following commutator between an odd operator and an operator defined on a direct sum space,

$$
\begin{aligned}
&[(r\lambda i(x_1\lambda_1, x_1\lambda_1)), (r'\lambda' i'(x_1\lambda_1, x_2\lambda_2))] \\
&\qquad = \sum_{\lambda_3} (|\lambda||\lambda'||\lambda_3|)^{\frac{1}{2}} (\lambda\lambda'\lambda_3)_{r_4 ii'}{}^{j} \left\{ \begin{pmatrix} \lambda & \lambda' & \lambda_3 \\ \lambda_2 & \lambda_1 & \lambda_1 \end{pmatrix} \right\}_{rr'r_3r_4} \\
&\qquad\quad \times \theta(\lambda_1\lambda\lambda_1 r)\theta(\lambda_1\lambda'\lambda_2 r')(r_3\lambda_3 j(x_1\lambda_1, x_2\lambda_2))
\end{aligned}
\tag{19}
$$

where $(x_1\lambda_1) \neq (x_2\lambda_2)$. From this it is clear that the commutator of an odd operator defined on $\lambda_1 \otimes \lambda_1$ and an operator defined on $\lambda_1 \otimes \lambda_2$ is a linear combination of operators defined on $\lambda_1 \otimes \lambda_2$. Hence, the operators defined on $\lambda_1 \otimes \lambda_2$ are closed under commutation with

Table 1. Kronecker products for the icosahedral group. Symmetrized and antisymmetrized products are indicated as $[\,]_S$ and $\{\}_A$, respectively.

		Product with				
Irrep	$\|\Gamma\|$	A	T_1	T_2	G	H
A	1	$[A]_S$	T_1	T_2	G	H
T_1	3		$[A+H]_S + \{T_1\}_A$	$G+H$	T_2+G+H	T_1+T_2+G+H
T_2	3			$[A+H]_S + \{T_2\}_A$	T_1+G+H	T_1+T_2+G+H
G	4				$[A+G+H]_S + \{T_1+T_2\}_A$	T_1+T_2+G+2H
H	5					$[A+G+2H]_S + \{T_1+T_2+G\}_A$

the odd operators, and will again carry irreps of the continuous group (G_1 say) generated by the odd operators.

Under the action of the odd operators defined on $\lambda_2 \otimes \lambda_2$ the following commutator occurs,

$$[(r\lambda i(x_2\lambda_2, x_2\lambda_2)), (r'\lambda' i'(x_1\lambda_1, x_2\lambda_2))]$$
$$= -\sum_{\lambda_3}(|\lambda||\lambda'||\lambda_3|)^{\frac{1}{2}}(\lambda'\lambda\lambda_3)_{r_4 i' i}{}^{j} \begin{Bmatrix} \lambda' & \lambda & \lambda_3 \\ \lambda_2 & \lambda_1 & \lambda_2 \end{Bmatrix}_{r'rr_3r_4} \quad (20)$$
$$\times\theta(\lambda_1\lambda'\lambda_2 r')\theta(\lambda_2\lambda\lambda_2 r)(r_3\lambda_3 j(x_1\lambda_1, x_2\lambda_2)).$$

The operators defined on $\lambda_1 \otimes \lambda_2$ are also closed under commutation with the odd operators defined on $\lambda_2 \otimes \lambda_2$. Hence, these odd operators generate a continuous group (G_2 say), with the $\lambda_1 \otimes \lambda_2$ operators carrying irreps of this group. It is clear that the generators of G_1 commute with the generators of G_2 so that the $\lambda_1 \otimes \lambda_2$ operators above also carry irreps for the continuous group $G_1 \otimes G_2$. Using these results it is possible to generate many higher-order rotation groups associated with the electronic spaces $(T_1 \oplus T_2)$, $(T_i \oplus G)$, $(T_i \oplus H)$ and $(G \oplus H)$. If the $\lambda_1 \otimes \lambda_2$ electronic operators are associated with vibrational modes that transform in the same manner, a linear JT Hamiltonian may be formed that is invariant under the continuous group operations.

The results of Pooler [11] describing the groups generated by odd operators defined on single irrep spaces may now be used to determine the continuous groups that are carried by the $\lambda_1 \otimes \lambda_2$ operators defined on the direct sum spaces. The rotational groups that may be generated are as follows.

For the $(T_1 \oplus T_2)$ direct sum space,

$$(T_1 \oplus T_2) \otimes (T_1 \oplus T_2) = (T_1 \otimes T_1) \oplus (T_2 \otimes T_2) \oplus (T_1 \otimes T_2) \oplus (T_2 \otimes T_1)$$
$$= ([A \oplus H]_{\mathrm{S}} \oplus \{T_1\}_{\mathrm{A}}) \oplus ([A \oplus H]_{\mathrm{S}} \oplus \{T_2\}_{\mathrm{A}}) \oplus 2(G \oplus H). \quad (21)$$

The odd operators, transforming as T_1 and T_2, each generate the group SO(3). This means that it is possible to form Hamiltonians with SO(3) or SO(4) symmetry.

Similarly for the $(T_i \oplus G)$ direct sum space, the two sets of generators are T_i (which generates SO(3)) and $T_1 \oplus T_2$ which may generate SO(3) or SO(4). Hence there are three types of Hamiltonian which may be constructed, SO(3), SO(4) and SO(3) $\otimes$ SO(4).

For the $(T_i \oplus H)$ space the two sets of generators are T_i and $T_1 \oplus T_2 \oplus G$ which generates either SO(3) or SO(5). Hence, there are four possible types of Hamiltonian, SO(3), SO(4), SO(5) and SO(3) $\otimes$ SO(5).

For the $(G \oplus H)$ space the two sets of generators are $T_1 \oplus T_2$ and $T_1 \oplus T_2 \oplus G$. Hence, there are six possible types of Hamiltonian, SO(3), SO(4), SO(5), SO(3) $\otimes$ SO(4), SO(3) $\otimes$ SO(5) and SO(4) $\otimes$ SO(5).

These results are summarized in table 2. The way in which the icosahedral irreps embed in irreps of the continuous groups is also indicated. The notation for the irrep labels of $G_1 \otimes G_2$ will be explained in section 5 for each case.

It is also clearly possible to consider larger direct sums of irreducible electronic spaces. However, as any $\lambda_1 \otimes \lambda_2$ irrep operator is made up of ket–bras from at most two different irreducible spaces, there will only be non-zero commutation relations for any given $\lambda_1 \otimes \lambda_2$ operator with at most two sets of group generators. Studying the group behaviour of all the 'two irrep' direct sum spaces will provide all the information needed to characterize the larger direct sum spaces.

In the following section the continuous groups that may be generated on the electronic spaces $T_1 \oplus T_2$, $T_i \oplus G$, $T_i \oplus H$ and $G \oplus H$ will be discussed. The notation $(r\Lambda\lambda(\Gamma_1, \Gamma_2))$

Table 2. The continuous groups generated on the direct sum electronic spaces in icosahedral linear Jahn–Teller systems. (The notation T_i and T_j indicates that within a row of the table if $i = 1$ then $j = 2$ and *vice versa*.)

System	Group	Embedding $G_1 \otimes G_2 \supset I$
$(T_1 \oplus T_2) \otimes (g \oplus h)$	SO(3) ⊗ SO(3)	$(11) \equiv g \oplus h$
$(T_i \oplus G) \otimes (t_j \oplus g \oplus h)$	SO(3) ⊗ SO(4)	$(1(\frac{1}{2}\frac{1}{2})) \equiv t_j \oplus g \oplus h$
$(T_i \oplus H) \otimes (t_1 \oplus t_2 \oplus g \oplus h)$	SO(3) ⊗ SO(5)	$(1[10]) \equiv t_1 \oplus t_2 \oplus g \oplus h$
$(G \oplus H) \otimes (t_1 \oplus t_2 \oplus g \oplus 2h)$	SO(4) ⊗ SO(5)	$((\frac{1}{2}\frac{1}{2})[10]) \equiv t_1 \oplus t_2 \oplus g \oplus {}^1h \oplus {}^2h$

will be used to indicate an irreducible tensor operator transforming as the basis function λ of the irrep Λ and built on the electronic ket–bra set $|\Gamma_1\gamma\rangle\langle\Gamma_2\gamma_2'|$. Where there is no ambiguity the more compact notation $J_\lambda^{r\Lambda}$ will also be used.

5. The linear JT Hamiltonians of the electronic spaces $T_1 \oplus T_2$, $T_i \oplus G$, $T_i \oplus H$ and $G \oplus H$

5.1. The $T_1 \oplus T_2$ system

From (21) it is clear that the group generators for the $(T_1 \oplus T_2)$ direct sum problem will be the electronic operators transforming as the odd irreps T_1 and T_2. Within their respective Kronecker product spaces, $T_1 \otimes T_1$ and $T_2 \otimes T_2$, these generators act in the manner described by Pooler, generating SO(3) symmetry. It will now be of interest to consider the operators existing in the $T_1 \otimes T_2$ and $T_2 \otimes T_1$ product spaces as these will carry non-trivial irreps of the larger continuous group referred to generally as $G_1 \otimes G_2$ in section 4.

The six odd operators may be written as

$$\begin{array}{ll} (T_1 + 1(T_1, T_1)) & (T_2 + 2(T_2, T_2)) \\ (T_1 \quad 0(T_1, T_1)) & (T_2 \quad 0(T_2, T_2)) \\ (T_1 - 1(T_1, T_1)) & (T_2 - 2(T_2, T_2)) \end{array} \tag{22}$$

where the numerical labelling of the basis within an irrep is that of Pooler [10] and the operator notation follows (15). Generators of SO(3) and SO(4) may now be defined,

$$\begin{array}{ll} S_0 = -\sqrt{2}i(T_1 \quad 0(T_1, T_1)) & L_0 = -\sqrt{2}i(T_2 \quad 0(T_2, T_2)) \\ S_\pm = \quad 2i(T_1 \pm 1(T_1, T_1)) & L_\pm = \quad 2i(T_2 \mp 2(T_2, T_2)) \end{array} \tag{23}$$

where $(S_\pm, S_0)$ and $(L_\pm, L_0)$ separately satisfy the usual SO(3) commutation relations and also commute with each other.

Under commutation with the non-shift operators (S_0, L_0) the highest weights may be found for each type of electronic operator. The irreps of SO(4) may then be associated with the electronic operators as follows:

$$\begin{array}{llll} (10) \to T_1 & (01) \to T_2 & (00) \to A & (20) \to H \\ & (02) \to H & (11) \to G \oplus H & \end{array} \tag{24}$$

(where $(s_i l_i)$ indicates the highest eigenvalues of S_0, L_0 for a given irrep) so that (21) may be written

$$\{(10) \oplus (01)\} \otimes \{(10) \oplus (01)\} = \{(00) \oplus (20) \oplus (10)\} \oplus \{(00) \oplus (02) \oplus (01)\} \oplus 2(11). \tag{25}$$

The $G \oplus H$ operators defined on $T_1 \otimes T_2$ and $T_2 \otimes T_1$ carry the irrep (11) of SO(4).

In the following work the notation $J_i^H \equiv (H \quad i(T_1, T_2))$ or $(H \quad i(T_2, T_1))$ will be used for brevity, with a similar expression for the G operators. The labelling of the basis within an irrep is again that of Pooler. In constructing an invariant Hamiltonian it is possible to use the operators $(\lambda \quad i(T_1, T_2))$ or $(\lambda \quad i(T_2, T_1))$. The icosahedral operators embed in the (11) irrep of SO(4) in the same way for each case, so that it is not necessary to specify which set is being used when considering the formation of the invariant Hamiltonians.

From the observation that $[S_0, J_0^H] = 0$ and $[L_0, J_0^H] = 0$ it is seen that J_0^H transforms as the $(0, 0)$ component of some SO(4) irrep. Using the $S_\pm$ and $L_\pm$ generators it is possible under commutation to produce all the other components of the irrep as well as demonstrating that $(1, 1)$ is the highest weight so that (11) labels the irrep. The operators carrying the (11) irrep are expressed in terms of the icosahedral operators as follows:

$$J_{11}^{(11)} = \frac{1}{\sqrt{3}}(\sqrt{2}J_{-1}^H - iJ_{-1}^G) \qquad J_{01}^{(11)} = \frac{1}{\sqrt{3}}(J_{-2}^H - \sqrt{2}iJ_{-2}^G)$$
$$J_{10}^{(11)} = \frac{1}{\sqrt{3}}(-J_1^H + \sqrt{2}iJ_1^G)$$
$$J_{-11}^{(11)} = \frac{1}{\sqrt{3}}(\sqrt{2}J_2^H - iJ_2^G) \qquad J_{1-1}^{(11)} = \frac{1}{\sqrt{3}}(\sqrt{2}J_{-2}^H + iJ_{-2}^G)$$
$$J_{-10}^{(11)} = \frac{1}{\sqrt{3}}(J_{-1}^H + \sqrt{2}iJ_{-1}^G)$$
$$J_{0-1}^{(11)} = \frac{1}{\sqrt{3}}(-J_2^H - \sqrt{2}iJ_2^G) \qquad J_{-1-1}^{(11)} = \frac{1}{\sqrt{3}}(\sqrt{2}J_1^H + iJ_1^G) \qquad J_{00}^{(11)} = J_0^H. \tag{26}$$

It is also of interest to construct a set of operators transforming as irreps of the SO(3) group under one set of SO(3) generators. As a particular example, the S generators are chosen in what follows. The L generators could equally have been chosen.

Under the action of the S generators it is possible to divide the nine basis operators of the (11) irrep into three SO(3) irreps with weight 1

$$\begin{array}{lclcl} T_0^{(1)} = J_{00}^{(11)} & & \tilde{T}_0^{(1)} = J_{01}^{(11)} & & \tilde{\tilde{T}}{}_0^{(1)} = J_{0-1}^{(11)} \\ T_1^{(1)} = J_{10}^{(11)} & \text{and} & \tilde{T}_1^{(1)} = J_{11}^{(11)} & \text{and} & \tilde{\tilde{T}}{}_1^{(1)} = J_{1-1}^{(11)} \\ T_{-1}^{(1)} = J_{-10}^{(11)} & & \tilde{T}_{-1}^{(1)} = J_{-11}^{(11)} & & \tilde{\tilde{T}}{}_{-1}^{(1)} = J_{-1-1}^{(11)}. \end{array} \tag{27}$$

It is found, however, that if the three possible SO(3) invariant Hamiltonians $\{T^{(1)}Q^{(1)}\}_0^0$, $\{\tilde{T}^{(1)}\tilde{Q}^{(1)}\}_0^0$ and $\{\tilde{\tilde{T}}{}^{(1)}\tilde{\tilde{Q}}{}^{(1)}\}_0^0$ are formed, their sum does not produce the form of the icosahedral invariant $G \oplus H$ Hamiltonian. Instead, if linear combinations of the nine SO(3) operators are taken, it is possible to produce three weight 1 SO(3) irreps whose invariant Hamiltonians may be combined to give the equal coupling icosahedral invariant $G \oplus H$ Hamiltonian. These linear combinations may be expressed as

$$\begin{aligned} H_i^{(1)+} &= \frac{1}{\sqrt{2}}\left(J_{i0}^{(11)} + \frac{1}{\sqrt{2}}(J_{i1}^{(11)} - J_{i-1}^{(11)})\right) \\ H_i^{(1)-} &= \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(J_{i1}^{(11)} - J_{i-1}^{(11)}) - J_{i0}^{(11)}\right) \\ T_i^{(1)'} &= \frac{1}{\sqrt{2}}(J_{i1}^{(11)} + J_{i-1}^{(11)}) \end{aligned} \tag{28}$$

where $i = \pm 1, 0$ in each case and in (28) $H^{(1)+}$ and $H^{(1)-}$ are two weight 1 SO(3) irreps (the H here does not refer to icosahedral irrep labelling). Using these operators then the

Hamiltonians invariant under SO(4), SO(3) and I are related respectively by

$$
\begin{aligned}
3\{J^{(11)}Q^{(11)}\}^{(00)}_{00} &= \sqrt{3}(\{T^{(1)'}Q^{(1)'}\}^{(0)}_0 - \{H^{(1)+}Q^{(1)+}\}^{(0)}_0 - \{H^{(1)-}Q^{(1)-}\}^{(0)}_0) \\
&= \sqrt{5}\{J^H Q^H\}^A_0 + 2\{J^G Q^G\}^A_0
\end{aligned}
\tag{29}
$$

where from the general tensor coupling relation of (5)

$$
\begin{aligned}
&\sum_{m_1,m_2}(-1)^{j_1-m_1}(-1)^{j_2-m_2}J^{(j_1j_2)}_{m_1m_2}Q^{(j_1j_2)}_{-m_1-m_2} = \{J^{(j_1j_2)}Q^{(j_1j_2)}\}^{(00)}_{00}(|j_1||j_2|)^{\frac{1}{2}} \\
&\sum_m(-1)^{j-m}J^{(j)}_m Q^{(j)}_{-m} = \{J^{(j)}Q^{(j)}\}^{(0)}_0|j|^{\frac{1}{2}} \\
&\sum_i J^\lambda_i Q^\lambda_{-i} = \{J^\lambda Q^\lambda\}^A_0|\lambda|^{\frac{1}{2}}.
\end{aligned}
\tag{30}
$$

Hence, it is possible to create a $(T_1 \oplus T_2) \otimes (g \oplus h)$ linear JT Hamiltonian that is simultaneously invariant under SO(4) and SO(3) as well as I.

5.2. The $T_1 \oplus G$ and $T_2 \oplus G$ systems

5.2.1. $T_1 \oplus G$. Consider the Kronecker product,

$$
\begin{aligned}
(T_1 \oplus G) \otimes (T_1 \oplus G) &= (T_1 \otimes T_1) \oplus (G \otimes G) \oplus (T_1 \otimes G) \oplus (G \otimes T_1) \\
&= ([A \oplus H]_{\mathrm{S}} \oplus \{T_1\}_{\mathrm{A}}) \oplus ([A \oplus G \oplus H]_{\mathrm{S}} \oplus \{T_1 \oplus T_2\}_{\mathrm{A}}) \oplus 2(T_2 \oplus G \oplus H).
\end{aligned}
\tag{31}
$$

From this it is clear that the generators for the problem will be the T_1 operators within the $T_1 \otimes T_1$ product space and the T_1 and T_2 operators within the $G \otimes G$ product space. Pooler [11] demonstrated that these generate the groups SO(3) and SO(4) respectively; hence the operators defined on the product space $T_1 \otimes G$ or $G \otimes T_1$ will, from the discussion in section 4, carry irreps of the group SO(3) $\otimes$ SO(4).

The generators of SO(3) and SO(4) may be written

$$
\begin{aligned}
&J_0 = -\sqrt{2}i(T_1\ 0(T_1, T_1)) \qquad L_0 = i(T_2\ 0(G, G)) \qquad S_0 = i(T_1\ 0(G, G)) \\
&J_\pm = 2i(T_1 \pm 1(T_1, T_1)) \qquad L_\pm = \sqrt{2}i(T_2 \pm 2(G, G)) \qquad S_\pm = \sqrt{2}i(T_1 \pm 1(G, G))
\end{aligned}
\tag{32}
$$

where $(J_0, J_\pm)$, $(L_0, L_\pm)$ and $(S_0, S_\pm)$ separately satisfy the usual SO(3) commutation relations and also commute with each other.

Under commutation with the non-shift operators (J_0, L_0, S_0) the highest weights may be found for each type of electronic operator. The irreps of SO(3) $\otimes$ SO(4) may then be associated with the icosahedral irreps as follows:

$$
\begin{aligned}
&(1(00)) \rightarrow T_1 \qquad (0(00)) \rightarrow A \qquad (2(00)) \rightarrow H \qquad (0(11)) \rightarrow G \oplus H \\
&(0(10)) \rightarrow T_1 \qquad (0(01)) \rightarrow T_2 \qquad (0(\tfrac{1}{2}\tfrac{1}{2})) \rightarrow G \\
&\qquad (1(\tfrac{1}{2}\tfrac{1}{2})) \rightarrow T_2 \oplus G \oplus H
\end{aligned}
\tag{33}
$$

(where $(j_i(l_is_i))$ indicates the highest eigenvalues of (J_0, L_0, S_0) for a given irrep) so that (31) may be written

$$
\begin{aligned}
&\{(1(00)) \oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \otimes \{(1(00)) \oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \\
&\qquad = \{(0(00)) \oplus (2(00)) \oplus (1(00))\} \oplus \{(0(00)) \oplus (0(11)) \oplus (0(10)) \oplus (0(01))\} \\
&\qquad\quad \oplus 2(1(\tfrac{1}{2}\tfrac{1}{2})).
\end{aligned}
\tag{34}
$$

The $T_2 \oplus G \oplus H$ operators defined on $T_1 \otimes G$ or $G \otimes T_1$ carry the irrep $(1(\frac{1}{2}\frac{1}{2}))$ of $SO(3) \otimes SO(4)$.

The embedding of the icosahedral operators T_2, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is given in section A.3 of the appendix both for operators defined on the (T_1, G) and (G, T_1) ket–bra basis where the notation $J_i^\Lambda = (\Lambda i(T_1, G))$ and $J_i^\Lambda = (\Lambda i(G, T_1))$ is adopted for brevity there and in what now follows.

Using the operators given in section A.3, the Hamiltonians invariant under $SO(3) \otimes SO(4)$ and I are related by,

$$2\sqrt{3}\{J^{(1(\frac{1}{2}\frac{1}{2}))}Q^{(1(\frac{1}{2}\frac{1}{2}))}\}_{000}^{(0(00))} = \sqrt{5}\{J^H Q^H\}_0^A + 2\{J^G Q^G\}_0^A + \sqrt{3}\{J^{T_2} Q^{T_2}\}_0^A \tag{35}$$

where

$$\begin{aligned}\sum_{m_1,m_2,m_3} &(-1)^{j_1-m_1}(-1)^{j_2-m_2}(-1)^{j_3-m_3} J_{m_1m_2m_3}^{(j_1j_2j_3)} Q_{-m_1-m_2-m_3}^{(j_1j_2j_3)} \\ &= \{J^{(j_1j_2j_3)}Q^{(j_1j_2j_3)}\}_{000}^{(000)}(|j_1||j_2||j_3|)^{\frac{1}{2}}\end{aligned} \tag{36}$$

and

$$\sum_i J_i^\lambda Q_{-i}^\lambda = \{J^\lambda Q^\lambda\}_0^A |\lambda|^{\frac{1}{2}}. \tag{37}$$

Hence, it is possible to create a $(T_1 \oplus G) \otimes (t_2 \oplus g \oplus h)$ linear JT Hamiltonian that is simultaneously invariant under $SO(3) \otimes SO(4)$ as well as I. This system may be expressed in the $SO(3) \otimes SO(4)$ notation as,

$$\{(1(00)) \oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \otimes (1(\tfrac{1}{2}\tfrac{1}{2})). \tag{38}$$

5.2.2. $T_2 \oplus G$. Consider the Kronecker product,

$$\begin{aligned}(T_2 \oplus G) \otimes (T_2 \oplus G) &= (T_2 \otimes T_2) \oplus (G \otimes G) \oplus (T_2 \otimes G) \oplus (G \otimes T_2) \\ &= ([A \oplus H]_S \oplus \{T_2\}_A) \oplus ([A \oplus G \oplus H]_S \oplus \{T_1 \oplus T_2\}_A) \\ &\quad \oplus 2(T_1 \oplus G \oplus H).\end{aligned} \tag{39}$$

From this it is clear that the generators for the problem will be the T_2 operators within the $T_2 \otimes T_2$ product space and the T_1 and T_2 operators within the $G \otimes G$ product space. Pooler [11] demonstrated that the T_2 operators generate the group SO(3), hence the operators defined on the product space $T_2 \otimes G$ or $G \otimes T_2$ will, from the discussion in section 4, carry irreps of the group $SO(3) \otimes SO(4)$.

The SO(4) generators have been given in section 5.2.1 and the SO(3) generators in section 5.1 may be written

$$\begin{aligned}J_0 &= -\sqrt{2}i(T_2\, 0(T_2, T_2)) \\ J_\pm &= 2i(T_2 \mp 2(T_2, T_2)).\end{aligned} \tag{40}$$

Under commutation with the non-shift operators (J_0, L_0, S_0) the highest weights may be found for each type of electronic operator. The irreps of $SO(3) \otimes SO(4)$ may then be associated with the icosahedral irreps as follows,

$$\begin{array}{llll}(1(00)) \to T_2 & (0(00)) \to A & (2(00)) \to H & (0(11)) \to G \oplus H \\ (0(10)) \to T_1 & (0(01)) \to T_2 & (0(\frac{1}{2}\frac{1}{2})) \to G & (1(\frac{1}{2}\frac{1}{2})) \to T_1 \oplus G \oplus H\end{array} \tag{41}$$

so that (39) may be written

$$\begin{aligned}\{(1(00)) &\oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \otimes \{(1(00)) \oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \\ &= \{(0(00)) \oplus (2(00)) \oplus (1(00))\} \oplus \{(0(00)) \oplus (0(11)) \oplus (0(10)) \oplus (0(01))\} \\ &\quad \oplus 2(1(\tfrac{1}{2}\tfrac{1}{2})).\end{aligned} \tag{42}$$

The $T_1 \oplus G \oplus H$ operators defined on $T_2 \otimes G$ or $G \otimes T_2$ carry the irrep $(1(\frac{1}{2}\frac{1}{2}))$ of SO(3) $\otimes$ SO(4).

The embedding of the icosahedral operators T_1, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is given in section A.3 both for the operators defined on the (T_2, G) and (G, T_2) ket–bra basis where the notation $J_i^\Lambda = (\Lambda i(T_2, G))$ and $J_i^\Lambda = (\Lambda i(G, T_2))$ is adopted for brevity there and in what now follows.

Using the operators defined in section A.3, the Hamiltonians invariant under SO(3) $\otimes$ SO(4) and I are related by

$$2\sqrt{3}\{J^{(1(\frac{1}{2}\frac{1}{2}))}Q^{(1(\frac{1}{2}\frac{1}{2}))}\}_{000}^{(0(00))} = \sqrt{5}\{J^H Q^H\}_0^A + 2\{J^G Q^G\}_0^A + \sqrt{3}\{J^{T_1}Q^{T_1}\}_0^A. \tag{43}$$

Hence, it is possible to create a $(T_2 \oplus G) \otimes (t_1 \oplus g \oplus h)$ linear JT Hamiltonian that is simultaneously invariant under SO(3) $\otimes$ SO(4) as well as I. This system may (as with the $(T_1 \oplus G)$ model) be expressed in the SO(3) $\otimes$ SO(4) notation as

$$\{(1(00)) \oplus (0(\tfrac{1}{2}\tfrac{1}{2}))\} \otimes (1(\tfrac{1}{2}\tfrac{1}{2})). \tag{44}$$

5.3. The $T_1 \oplus H$ and $T_2 \oplus H$ systems

5.3.1. $(T_1 \oplus H)$. Consider the Kronecker product,

$$\begin{aligned}(T_1 \oplus H) \otimes (T_1 \oplus H) &= (T_1 \otimes T_1) \oplus (H \otimes H) \oplus (T_1 \otimes H) \oplus (H \otimes T_1)\\ &= ([A \oplus H]_S \oplus \{T_1\}_A) \oplus ([A \oplus {}^2G \oplus {}^1H \oplus {}^2H]_S\\ &\quad \oplus\{T_1 \oplus T_2 \oplus {}^1G\}_A) \oplus 2(T_1 \oplus T_2 \oplus G \oplus H)\end{aligned} \tag{45}$$

where the multiplicity labels of Pooler [11] have been used in the $H \otimes H$ product.

From this it is clear that the generators for the problem will be the T_1 operators within the $T_1 \otimes T_1$ product space and the T_1, T_2 and G operators within the $H \otimes H$ product space. Pooler [11] demonstrated that the generators within the $H \otimes H$ space generate the group SO(5); hence the operators defined on the product space $T_1 \otimes H$ or $H \otimes T_1$ will, from the discussion in section 4, carry irreps of the group SO(3) $\otimes$ SO(5). The generators of the SO(3) group were given in section 5.2. Using a result of Pooler ([11] equation (4.4)) which derives from the work of Judd [6], the generators of the group SO(5) may be expressed in the Cartan–Weyl basis as

$$\begin{aligned}W_{\gamma\gamma'} &= \sum_{r\Lambda\lambda}(1 - \theta(HH\Lambda r))[\Lambda]^{\frac{1}{2}} \begin{pmatrix} H & \lambda & \gamma' \\ \gamma & \Lambda & H \end{pmatrix}^r (r\Lambda\lambda(H, H))\\ &= |H\gamma\rangle\langle H\gamma'| - |H - \gamma'\rangle\langle H - \gamma|\end{aligned} \tag{46}$$

where the sum is over the odd irreps of the $H \otimes H$ Kronecker product. There are two non-shift operators, W_{22} and W_{11}, whose eigenvalues may be used to characterize irreps of the group SO(5). The basis within an irrep may be specified by the pair of eigenvalues of (W_{22}, W_{11}) which is otherwise known as the 'weight'. The irrep as a whole is specified by giving the 'highest' weight associated with a basis state within the irrep. (A weight $(w_1 w_2)$ is 'higher' than a weight $(w_1' w_2')$ if $w_1 > w_1'$ or if $w_1 = w_1'$, $w_2 \geqslant w_2'$.) The $W_{\gamma\gamma'}$ are not linearly independent as $W_{-\gamma'-\gamma} = -W_{\gamma\gamma'}$. The following set of generators in addition to the two non-shift operators, W_{22} and W_{11}, form a linearly independent set which generates the group SO(5),

$$\begin{aligned}&W_{+-} = W_{21} \qquad W_{--} = W_{-12} \qquad W_{0-} = W_{01} \qquad W_{+0} = W_{20}\\ &W_{++} = W_{2-1} \qquad W_{-+} = W_{12} \qquad W_{0+} = W_{10} \qquad W_{-0} = W_{02}.\end{aligned} \tag{47}$$

In the above, the way in which each shift operator affects the weight of a state on which it acts has been indicated, with $+$, $-$ and 0 indicating a change in the weight of $+1$, -1 and 0, respectively.

Under commutation with the non-shift operators (J_0, W_{22}, W_{11}) the highest weights may be found for each type of electronic operator. The irreps of $SO(3) \otimes SO(5)$ may then be associated with the icosahedral irreps as follows:

$$
\begin{aligned}
&(0[00]) \rightarrow A \qquad (2[00]) \rightarrow H \qquad (1[00]) \rightarrow T_1 \\
&(0[10]) \rightarrow H \qquad (0[20]) \rightarrow {}^2G \oplus {}^1H \oplus {}^2H \qquad (0[11]) \rightarrow T_1 \oplus T_2 \oplus {}^1G \\
&(1[10]) \rightarrow T_1 \oplus T_2 \oplus G \oplus H
\end{aligned} \tag{48}
$$

(where $(j_i[w_{22i} w_{11i}])$ indicates the highest eigenvalues of (J_0, W_{22}, W_{11}) for a given irrep) so that (45) may be written

$$
\begin{aligned}
&\{(1[00]) \oplus (0[10])\} \otimes \{(1[00]) \oplus (0[10])\} \\
&\qquad = \{(0[00]) \oplus (2[00]) \oplus (1[00])\} \oplus \{(0[00]) \oplus (0[20]) \oplus (0[11])\} \oplus 2(1[10]).
\end{aligned} \tag{49}
$$

The $T_1 \oplus T_2 \oplus G \oplus H$ operators defined on $T_1 \otimes H$ or $H \otimes T_1$ carry the irrep (1[10]) of $SO(3) \otimes SO(5)$.

The embedding of the icosahedral operators T_1, T_2, G and H in the irrep (1[10]) is given in section A.4 both for the operators defined on the (T_1, H) and (H, T_1) ket–bra basis where the notation $J_i^\Lambda = (\Lambda i(T_1, H))$ and $J_i^\Lambda = (\Lambda i(H, T_1))$ is adopted for brevity there and in what now follows.

Using the operators given in section A.4, the Hamiltonians invariant under $SO(3) \otimes SO(5)$ and I are related by

$$
\begin{aligned}
&\sqrt{15}\{J^{(1[10])} Q^{(1[10])}\}_{000}^{(0[00])} \\
&\qquad = (\sqrt{5}\{J^H Q^H\}_0^A + 2\{J^G Q^G\}_0^A + \sqrt{3}\{J^{T_1} Q^{T_1}\}_0^A + \sqrt{3}\{J^{T_2} Q^{T_2}\}_0^A).
\end{aligned} \tag{50}
$$

The $SO(3) \otimes SO(5)$ invariant is constructed by taking the product of an SO(3) invariant with an SO(5) invariant as follows,

$$\sqrt{15}\{J^{(1[10])} Q^{(1[10])}\}_{000}^{(0[00])} = \sqrt{3}\{J^{(1)} Q^{(1)}\}_0^{(0)} \sqrt{5}\{J^{[10]} Q^{[10]}\}_{00}^{[00]} \tag{51}$$

where

$$\sum_m (-1)^{j-m} J_m^{(j)} Q_{-m}^{(j)} = \{J^{(j)} Q^{(j)}\}_0^{(0)} |j|^{\frac{1}{2}} \tag{52}$$

$$\{J^{[10]} Q^{[10]}\}_{00}^{[00]} = \sum_{\alpha_1,\beta_1,\alpha_2,\beta_2} \langle [10](\alpha_1\beta_1); [10](\alpha_2\beta_2) | [00](00) \rangle J_{\alpha_1\beta_1}^{[10]} Q_{\alpha_2\beta_2}^{[10]} \tag{53}$$

and an $SO(3) \otimes SO(5)$ operator is constructed out of the product of an SO(3) operator with an SO(5) operator,

$$J_{m_1 m_2 m_3}^{(j_1[j_2 j_3])} = J_{m_1}^{(j_1)} J_{m_2 m_3}^{[j_2 j_3]}. \tag{54}$$

In (53) the right-hand side contains the SO(5) Wigner coefficients. Hecht [5] expresses these Wigner coefficients as the product of a ‘double-barred’ Wigner coefficient with two ordinary SO(3) Wigner coefficients, and provides some tables of the double-barred Wigner coefficients including the ones involved in (53). In using the tables of Hecht it is necessary to transform to a different basis to the one used in the above work. The basis that has been used for the Cartan subalgebra in this paper is related to that of Hecht [5] via $J_0 = \frac{1}{2}(W_{22} + W_{11})$

and $\Lambda_0 = \frac{1}{2}(W_{22} - W_{11})$. Using the tables of Hecht the SO(5) invariant in (53) may be expressed as

$$\sqrt{5}\{J^{[10]}Q^{[10]}\}^{[00]}_{00} = (J^{[10]}_{10}Q^{[10]}_{-10} + J^{[10]}_{-10}Q^{[10]}_{10} + J^{[10]}_{00}Q^{[10]}_{00} - J^{[10]}_{01}Q^{[10]}_{0-1} - J^{[10]}_{0-1}Q^{[10]}_{01}). \quad (55)$$

Hence, it is possible to create a $(T_1 \oplus H) \otimes (t_1 \oplus t_2 \oplus g \oplus h)$ linear JT Hamiltonian that is simultaneously invariant under SO(3) $\otimes$ SO(5) as well as I. This system may be expressed in the SO(3) $\otimes$ SO(5) notation as

$$\{(1[00]) \oplus (0[10])\} \otimes (1[10]). \quad (56)$$

5.3.2. $(T_2 \oplus H)$. Consider the Kronecker product,

$$\begin{aligned}(T_2 \oplus H) \otimes (T_2 \oplus H) &= (T_2 \otimes T_2) \oplus (H \otimes H) \oplus (T_2 \otimes H) \oplus (H \otimes T_2)\\ &= ([A \oplus H]_S \oplus \{T_2\}_A) \oplus ([A \oplus {}^2G \oplus {}^1H \oplus {}^2H]_S \\ &\quad \oplus \{T_1 \oplus T_2 \oplus {}^1G\}_A) \oplus 2(T_1 \oplus T_2 \oplus G \oplus H)\end{aligned} \quad (57)$$

where the multiplicity labels of Pooler [10] have been used in the $H \otimes H$ product.

From this it is clear that the generators for the problem will be the T_2 operators on the $T_2 \otimes T_2$ product space and the T_1, T_2 and G operators within the $H \otimes H$ product space; hence from sections 5.3.1 and 5.1 the operators defined on the product space $T_2 \otimes H$ or $H \otimes T_2$ will, from the discussion in section 4, carry irreps of the group SO(3) $\otimes$ SO(5).

Under commutation with the non-shift operators (J_0, W_{22}, W_{11}) (where J_0 now refers to the operator $-\sqrt{2}i(T_2\ 0(T_2, T_2))$ of (23)) the highest weights may be found for each type of electronic operator. The irreps of SO(3) $\otimes$ SO(5) may then be associated with the icosahedral irreps as follows:

$$\begin{aligned}&(0[00]) \to A \qquad (2[00]) \to H \qquad (1[00]) \to T_2\\ &(0[10]) \to H \qquad (0[20]) \to {}^2G \oplus {}^1H \oplus {}^2H \qquad (0[11]) \to T_1 \oplus T_2 \oplus {}^1G\\ &(1[10]) \to T_1 \oplus T_2 \oplus G \oplus H\end{aligned} \quad (58)$$

so that (57) may be written

$$\begin{aligned}&\{(1[00]) \oplus (0[10])\} \otimes \{(1[00]) \oplus (0[10])\}\\ &\quad = \{(0[00]) \oplus (2[00]) \oplus (1[00])\} \oplus \{(0[00]) \oplus (0[20]) \oplus (0[11])\} \oplus 2(1[10]).\end{aligned} \quad (59)$$

The $T_1 \oplus T_2 \oplus G \oplus H$ operators defined on $T_2 \otimes H$ or $H \otimes T_2$ carry the irrep (1[10]) of SO(3) $\otimes$ SO(5).

The embedding of the icosahedral operators T_1, T_2, G and H in the irrep (1[10]) is given in section A.4 both for the operators defined on the (T_2, H) and (H, T_2) ket–bra basis where the notation $J_i^\Lambda = (\Lambda i(T_2, H))$ and $J_i^\Lambda = (\Lambda i(H, T_2))$ is adopted for brevity there and in what now follows.

Using the operators given in section A.4, the Hamiltonians invariant under SO(3) $\otimes$ SO(5) and I are related by

$$\begin{aligned}&\sqrt{15}\{J^{(1[10])}Q^{(1[10])}\}^{(0[00])}_{000}\\ &\quad = (\sqrt{5}\{J^H Q^H\}^A_0 + 2\{J^G Q^G\}^A_0 + \sqrt{3}\{J^{T_1} Q^{T_1}\}^A_0 + \sqrt{3}\{J^{T_2} Q^{T_2}\}^A_0).\end{aligned} \quad (60)$$

Hence, it is possible to create a $(T_2 \oplus H) \otimes (t_1 \oplus t_2 \oplus g \oplus h)$ linear JT Hamiltonian that is simultaneously invariant under SO(3) $\otimes$ SO(5) as well as I. This system may (as with the $(T_1 \oplus H)$ model) be expressed in the SO(3) $\otimes$ SO(5) notation as

$$\{(1[00]) \oplus (0[10])\} \otimes (1[10]). \quad (61)$$

5.4. The $G \oplus H$ system

Consider the Kronecker product,

$$
\begin{aligned}
(G \oplus H) \otimes (G \oplus H) &= (G \otimes G) \oplus (H \otimes H) \oplus (G \otimes H) \oplus (H \otimes G) \\
&= ([A \oplus G \oplus H]_{\mathrm{S}} \oplus \{T_1 \oplus T_2\}_{\mathrm{A}}) \oplus ([A \oplus {}^2G \oplus {}^1H \oplus {}^2H]_{\mathrm{S}} \\
&\quad \oplus \{T_1 \oplus T_2 \oplus {}^1G\}_{\mathrm{A}}) \oplus 2(T_1 \oplus T_2 \oplus G \oplus {}^1H \oplus {}^2H). \qquad (62)
\end{aligned}
$$

From this it is clear that the generators for the problem will be the T_1 and T_2 operators within the $G \otimes G$ product space and the T_1, T_2 and G operators within the $H \otimes H$ product space. Hence, the operators defined on the product space $G \otimes H$ or $H \otimes G$ will, from the discussion in section 4, carry irreps of the group $SO(4) \otimes SO(5)$. The generators of SO(4) and SO(5) were given in sections 5.2 and 5.3, respectively.

Under commutation with the non-shift operators (L_0, S_0, W_{22}, W_{11}) the highest weights may be found for each type of electronic operator. The irreps of $SO(4) \otimes SO(5)$ may then be associated with the icosahedral irreps as follows,

$$
\begin{aligned}
&((00)[00]) \to A \qquad ((11)[00]) \to G \oplus H \qquad ((10)[00]) \to T_1 \\
&((01)[00]) \to T_2 \qquad ((\tfrac{1}{2}\tfrac{1}{2})[00]) \to G \qquad ((00[20]) \to {}^2G \oplus {}^1H \oplus {}^2H \\
&((00)[10]) \to H \qquad ((00)[11]) \to T_1 \oplus T_2 \oplus {}^1G \\
&\qquad ((\tfrac{1}{2}\tfrac{1}{2})[10]) \to T_1 \oplus T_2 \oplus G \oplus {}^1H \oplus {}^2H \qquad (63)
\end{aligned}
$$

so that (62) may be written

$$
\begin{aligned}
&\{((\tfrac{1}{2}\tfrac{1}{2})[00]) \oplus ((00)[10])\} \otimes \{((\tfrac{1}{2}\tfrac{1}{2})[00]) \oplus ((00)[10])\} \\
&\quad = \{((00)[00]) \oplus ((11)[00]) \oplus ((10)[00]) \oplus ((01)[00])\} \qquad (64) \\
&\quad\quad \oplus \{((00)[00]) \oplus ((00)[20]) \oplus ((00)[11])\} \oplus 2((\tfrac{1}{2}\tfrac{1}{2})[10]).
\end{aligned}
$$

The $T_1 \oplus T_2 \oplus G \oplus {}^1H \oplus {}^2H$ operators defined on $G \otimes H$ or $H \otimes G$ carry the irrep $((\tfrac{1}{2}\tfrac{1}{2})[10])$ of $SO(4) \otimes SO(5)$.

The embedding of the icosahedral operators T_1, T_2, G, ${}^1H$ and ${}^2H$ in the irrep $((\tfrac{1}{2}\tfrac{1}{2})[10])$ is given in the appendix section A.5 both for operators defined on the (G, H) and (H, G) ket–bra basis where the notation $J_i^{\Lambda} = (\Lambda i(G, H))$ and $J_i^{\Lambda} = (\Lambda i(H, G))$ is adopted for brevity there and in what now follows.

Using the operators given in section A.5, the Hamiltonians invariant under $SO(4) \otimes SO(5)$ and I are related by

$$
\begin{aligned}
&\sqrt{20}\{J^{((\frac{1}{2}\frac{1}{2})[10])} Q^{((\frac{1}{2}\frac{1}{2})[10])}\}^{((00)[00])}_{0000} \\
&\quad = \sqrt{3}\{J^{T_1} Q^{T_1}\}^A_0 + \sqrt{3}\{J^{T_2} Q^{T_2}\}^A_0 + 2\{J^G Q^G\}^A_0 + \sqrt{5}\{J^{{}^1H} Q^{{}^1H}\}^A_0 \\
&\quad\quad + \sqrt{5}\{J^{{}^2H} Q^{{}^2H}\}^A_0. \qquad (65)
\end{aligned}
$$

The $SO(4) \otimes SO(5)$ invariant is constructed by taking the product of an SO(4) invariant with an SO(5) invariant as follows,

$$
\sqrt{20}\{J^{((\frac{1}{2}\frac{1}{2})[10])} Q^{((\frac{1}{2}\frac{1}{2})[10])}\}^{((00)[00])}_{0000} = 2\{J^{(\frac{1}{2}\frac{1}{2})} Q^{(\frac{1}{2}\frac{1}{2})}\}^{(00)}_{00} \sqrt{5}\{J^{[10]} Q^{[00]}\}^{[00]}_{00} \qquad (66)
$$

where

$$
\sum_{m_1, m_2} (-1)^{j_1 - m_1} (-1)^{j_2 - m_2} J^{(j_1 j_2)}_{m_1 m_2} Q^{(j_1 j_2)}_{-m_1 -m_2} = \{J^{(j_1 j_2)} Q^{(j_1 j_2)}\}^{(00)}_{00} (|j_1||j_2|)^{\frac{1}{2}}. \qquad (67)
$$

Hence, it is possible to create a $(G \oplus H) \otimes (t_1 \oplus t_2 \oplus g \oplus {}^1h \oplus {}^2h)$ linear JT Hamiltonian that is simultaneously invariant under $SO(4) \otimes SO(5)$ as well as I. This system may be expressed in the $SO(4) \otimes SO(5)$ notation as

$$
\{((\tfrac{1}{2}\tfrac{1}{2})[00]) \oplus ((00)[10])\} \otimes ((\tfrac{1}{2}\tfrac{1}{2})[10]). \qquad (68)
$$

6. Conclusion

It has been shown that electronic operators may be defined upon an electronic space which is a direct sum of two or more irreducible spaces of a real character simple phase group (examples of which are the icosahedral group and the octahedral group) in such a way that there exist operators which are closed under commutation with a set of generators of a continuous group and hence carry irreps of that group. These operators are then coupled to a set of vibrational modes defined to transform in the same way, so that a JT Hamiltonian, which is invariant under simultaneous operations of the continuous group in electronic and vibrational space, is formed. This extends the work of Pooler [11] which considered operators defined on a single irreducible space. Within the icosahedral group the continuous groups generated on the two irrep direct sum spaces $(T_1 \oplus T_2)$, $(T_i \oplus G)$, $(T_i \oplus H)$ and $(G \oplus H)$ were presented in detail. JT systems of the type $(\Gamma_i \oplus \Gamma_j) \otimes \Sigma\lambda$ that may occur in the neutral C_{60} exciton spectrum exhibit these continuous group invariances and future work will exploit these additional group symmetries in order to treat the strong JT ground states of such systems analytically within the Born–Oppenheimer adiabatic approximation.

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Appendix

A.1. Derivation of equation (16)

Consider the transformation of the linear operator basis,

$$|x_1\lambda_1 i\rangle\langle x_2\lambda_2 i_2| \tag{69}$$

under the action of the group

$$\begin{aligned} O_R|x_1\lambda_1 i_1\rangle\langle x_2\lambda_2 i_2|O_{R^{-1}} &= O_R|x_1\lambda_1 i_1\rangle(O^\dagger_{R^{-1}}|x_2\lambda_2 i_2\rangle)^\dagger \\ &= \sum_{j_1 j_2}|x_1\lambda_1 j_1\rangle\langle x_2\lambda_2 j_2|\lambda(R)_{j_1 i_1}\lambda(R)^{j_2 i_2}. \end{aligned} \tag{70}$$

This is (15.2) of [1].

Using this equation, the transformation of the operator

$$(r\lambda i(x_1\lambda_1, x_2\lambda_2)) = |\lambda|^{\frac{1}{2}}(\lambda_1\lambda\lambda_2)_r{}^{i_1}{}_{ii_2}|x_1\lambda_1 i_1\rangle\langle x_2\lambda_2 i_2| \tag{71}$$

under the group action may be obtained. The left-hand side of (16) may be expressed as

$$\begin{aligned} &|\lambda|^{\frac{1}{2}}(\lambda_1\lambda\lambda_2)_r{}^{i_1}{}_{ii_2}O_R|x_1\lambda_1 i_1\rangle\langle x_2\lambda_2 i_2|O_{R^{-1}} \\ &\quad = |\lambda|^{\frac{1}{2}}(\lambda)^{i_1 j_1}(\lambda_1^*\lambda\lambda_2)_{rj_1 ii_2}\sum_{j_1' j_2'}|x_1\lambda_1 j_1'\rangle\langle x_2\lambda_2 j_2'|\lambda_1(R)_{j_1' i_1}\lambda_2(R)^{j_2' i_2} \end{aligned} \tag{72}$$

where the summation over j_1' and j_2' is made explicit for clarity. Using (4.4) of [1] and the unitarity of the 1-jm symbols it may be demonstrated that

$$(\lambda_1)^{i_1 j_1}\lambda_1(R)_{j_1' i_1} = (\lambda_1)^{j_1' i_1}\lambda_1^*(R)^{i_1 j_1}. \tag{73}$$

Inserting this result into (72) then the left-hand side of (16) becomes

$$= \sum_{j_1' j_2'} |\lambda|^{\frac{1}{2}} (\lambda_1)^{j_1' i_1} (\lambda_1^* \lambda \lambda_2)_{r j_1 i i_2} \lambda_1^*(R)^{i_1 j_1} \lambda_2(R)^{j_2' i_2} |x_1 \lambda_1 j_1'\rangle\langle x_2 \lambda_2 j_2'|. \tag{74}$$

Suppose that the result

$$(\lambda_1^* \lambda \lambda_2)_{r j_1 i i_2} \lambda_1^*(R)^{i_1 j_1} \lambda_2(R)^{j_2' i_2} = (\lambda_1^* \lambda \lambda_2)_{r i_1 j j_2'} \lambda(R)_{ji} \tag{75}$$

could be demonstrated. On substituting this into (74) and dropping the explicit j_1', j_2' summation, the result

$$|\lambda|^{\frac{1}{2}} (\lambda_1^* \lambda \lambda_2)_r{}^{j_1'}{}_{j j_2'} |x_1 \lambda_1 j_1'\rangle\langle x_2 \lambda_2 j_2'| \lambda(R)_{ji} = (r \lambda i (x_1 \lambda_1, x_2 \lambda_2)) \lambda(R)_{ji} \tag{76}$$

is obtained, which is precisely the right-hand side of (16). Thus to complete the proof, equation (75) must be demonstrated.

From (5.7) of [1],

$$(\lambda_1 \lambda_2 \lambda_3)_{r i_1 i_2 i_3} \lambda_1(R)_{i_1 j_1} \lambda_2(R)_{i_2 j_2} = \lambda_3(R)^{i_3 j_3} (\lambda_1 \lambda_2 \lambda_3)_{r j_1 j_2 j_3} \tag{77}$$

which is essentially a statement about the reducibility of a direct product of two irreps into a sum of irreps. Multiplying (77) by $\lambda_1(R)^{i_1' j_1}$ and summing over j_1 using the unitarity of the irrep matrices,

$$(\lambda_1 \lambda_2 \lambda_3)_{r i_1 i_2 i_3} \lambda_2(R)_{i_2 j_2} = \lambda_1(R)^{i_1 j_1} \lambda_3(R)^{i_3 j_3} (\lambda_1 \lambda_2 \lambda_3)_{r j_1 j_2 j_3} \tag{78}$$

which is precisely equation (75) and hence completes the proof.

A.2. Derivation of equation (18)

Consider the unitarity relation (5.6) of [1] for the 3-jm symbols,

$$\sum_{\lambda_3} |\lambda_3| (\lambda_1^* \lambda_2 \lambda_3)_{r j_1 j_2 j_3} (\lambda_1^* \lambda_2 \lambda_3)^{r j_1' j_2' j_3} = \delta_{j_1 j_1'} \delta_{j_2 j_2'}. \tag{79}$$

Multiplying both sides by $(\lambda_1)^{i_1 j_1} (\lambda_1)_{i_1' j_1'}$ and summing over j_1 and j_1' using (8.1) of [1], the unitarity of the 1-jm symbols and the theorem that the multiplicity tensor A_{rs} may always be chosen to equal δ_{rs} for groups for which (8.10) of [1] holds, the result,

$$\sum_{\lambda_3} |\lambda_3| (\lambda_1 \lambda_2 \lambda_3)_r{}^{j_1}{}_{j_2 j_3} (\lambda_1 \lambda_2 \lambda_3)_{r j_1'}{}^{j_2' j_3} = \delta_{j_1 j_1'} \delta_{j_2 j_2'} \tag{80}$$

is obtained. Multiplying (9.12) of [1] by $|\lambda_3| (\mu_1 \mu_2 \lambda_3)_{r_3 j_1'}{}^{j_2' i_3}$ and summing over λ_3, using (80), then the result,

$$(\lambda_1 \mu_2 \mu_3)_{r_1 i_1}{}^{j_2}{}_{j_3} (\mu_1 \lambda_2 \mu_3)_{r_2 j_1 i_2}{}^{j_3}$$
$$= \sum_{\lambda_3} |\lambda_3| (\mu_1 \mu_2 \lambda_3)_{r_3 j_1}{}^{j_2 i_3} (\lambda_1 \lambda_2 \lambda_3)_{r_4 i_1 i_2 i_3} \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \mu_1 & \mu_2 & \mu_3 \end{Bmatrix}_{r_1 r_2 r_3 r_4} \tag{81}$$

is obtained.

Clearly the left-hand side of (81) is related to parts of the right-hand side of (17). Permuting the columns on the left-hand side of (81) and using the fact that $\theta = \pm 1$ for simple phase groups,

$$(\mu_2 \lambda_1 \mu_3)_{r_1}{}^{j_2}{}_{i_1 j_3} (\mu_3 \lambda_2 \mu_1)_{r_2}{}^{j_3}{}_{i_2 j_1}$$
$$= \sum_{\lambda_3} |\lambda_3| (\mu_1 \mu_2 \lambda_3)_{r_3 j_1}{}^{j_2 i_3} (\lambda_1 \lambda_2 \lambda_3)_{r_4 i_1 i_2 i_3} \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \mu_1 & \mu_2 & \mu_3 \end{Bmatrix}_{r_1 r_2 r_3 r_4} \tag{82}$$
$$\times \theta(\mu_2^* \lambda_1 \mu_3 r_1) \theta(\mu_3^* \lambda_2 \mu_1 r_2).$$

Using the unitarity of the 1-jm symbols, the equation (8.1) of [1] and permuting columns, the result

$$(\mu_1\mu_2\lambda_3)_{r_3 j_1}{}^{j_2 i_3}(\lambda_1\lambda_2\lambda_3)_{r_4 i_1 i_2 i_3} = (\mu_2\lambda_3^*\mu_1)_{r_3}{}^{j_2}{}_{j j_1}(\lambda_1\lambda_2\lambda_3^*)_{r_4 i_1 i_2}{}^{j} \tag{83}$$

may be obtained, which when substituted into (82) produces the final result,

$$\begin{aligned}(\mu_2\lambda_1\mu_3)_{r_1}{}^{j_2}{}_{i_1 j_3}(\mu_3\lambda_2\mu_1)_{r_2}{}^{j_3}{}_{i_2 j_1} &= \sum_{\lambda_3}|\lambda_3|(\mu_2\lambda_3^*\mu_1)_{r_3}{}^{j_2}{}_{j j_1}(\lambda_1\lambda_2\lambda_3^*)_{r_4 i_1 i_2}{}^{j}\begin{Bmatrix}\lambda_1 & \lambda_2 & \lambda_3\\ \mu_1 & \mu_2 & \mu_3\end{Bmatrix}_{r_1 r_2 r_3 r_4}\\ &\quad\times\theta(\mu_2^*\lambda_1\mu_3 r_1)\theta(\mu_3^*\lambda_2\mu_1 r_2).\end{aligned} \tag{84}$$

In the case of a real character group, using this result in the right-hand side of (17) then (18) is obtained.

A.3. Embedding of the (T_1, G), (G, T_1), (T_2, G) and (G, T_2) icosahedral operators

A.3.1. (T_1, G). The embedding of the icosahedral operators T_2, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is as follows:

$$\begin{aligned}
&J^{(1(\frac12\frac12))}_{1\frac12\frac12} = \tfrac12(J^{T_2}_{-2} - \sqrt3 i J^{H}_{-2}) &&J^{(1(\frac12\frac12))}_{0\frac12\frac12} = \tfrac{1}{\sqrt6}(\sqrt3 J^{T_2}_{2} - \sqrt2 J^{G}_{2} - i J^{H}_{2})\\
&J^{(1(\frac12\frac12))}_{-1\frac12\frac12} = \tfrac{1}{\sqrt3}(-\sqrt2 J^{G}_{1} + i J^{H}_{1}) &&J^{(1(\frac12\frac12))}_{1\frac12-\frac12} = \tfrac{1}{2\sqrt3}(i J^{H}_{2} - 2\sqrt2 J^{G}_{2} - \sqrt3 J^{T_2}_{2})\\
&J^{(1(\frac12\frac12))}_{0\frac12-\frac12} = \tfrac{1}{\sqrt3}(-\sqrt2 i J^{H}_{1} - J^{G}_{1}) &&J^{(1(\frac12\frac12))}_{-1\frac12-\frac12} = \tfrac{1}{\sqrt2}(i J^{H}_{0} + J^{T_2}_{0})\\
&J^{(1(\frac12\frac12))}_{1-\frac12\frac12} = \tfrac{1}{\sqrt2}(i J^{H}_{0} - J^{T_2}_{0}) &&J^{(1(\frac12\frac12))}_{0-\frac12\frac12} = \tfrac{1}{\sqrt3}(\sqrt2 i J^{H}_{-1} - J^{G}_{-1})\\
&J^{(1(\frac12\frac12))}_{-1-\frac12\frac12} = \tfrac{1}{2\sqrt3}(i J^{H}_{-2} + 2\sqrt2 J^{G}_{-2} + \sqrt3 J^{T_2}_{-2}) &&J^{(1(\frac12\frac12))}_{1-\frac12-\frac12} = \tfrac{1}{\sqrt3}(-i J^{H}_{-1} - \sqrt2 J^{G}_{-1})\\
&J^{(1(\frac12\frac12))}_{0-\frac12-\frac12} = \tfrac{1}{\sqrt6}(-\sqrt3 J^{T_2}_{-2} + \sqrt2 J^{G}_{-2} - i J^{H}_{-2}) &&J^{(1(\frac12\frac12))}_{-1-\frac12-\frac12} = \tfrac12(\sqrt3 i J^{H}_{2} + J^{T_2}_{2})
\end{aligned} \tag{85}$$

where the notation $J^{\Lambda}_{i} = (\Lambda i(T_1, G))$ is adopted for brevity.

A.3.2. (G, T_1). The embedding of the icosahedral operators T_2, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is as follows:

$$\begin{aligned}
&J^{(1(\frac12\frac12))}_{1\frac12\frac12} = \tfrac12(J^{T_2}_{-2} + \sqrt3 i J^{H}_{-2}) &&J^{(1(\frac12\frac12))}_{0\frac12\frac12} = \tfrac{1}{\sqrt6}(\sqrt3 J^{T_2}_{2} + \sqrt2 J^{G}_{2} + i J^{H}_{2})\\
&J^{(1(\frac12\frac12))}_{-1\frac12\frac12} = \tfrac{1}{\sqrt3}(\sqrt2 J^{G}_{1} - i J^{H}_{1}) &&J^{(1(\frac12\frac12))}_{1\frac12-\frac12} = \tfrac{1}{2\sqrt3}(-\sqrt3 J^{T_2}_{2} + 2\sqrt2 J^{G}_{2} - i J^{H}_{2})\\
&J^{(1(\frac12\frac12))}_{0\frac12-\frac12} = \tfrac{1}{\sqrt3}(-\sqrt2 i J^{H}_{1} - J^{G}_{1}) &&J^{(1(\frac12\frac12))}_{-1\frac12-\frac12} = \tfrac{1}{\sqrt2}(-J^{T_2}_{0} + i J^{H}_{0})\\
&J^{(1(\frac12\frac12))}_{1-\frac12\frac12} = \tfrac{1}{\sqrt2}(J^{T_2}_{0} + i J^{H}_{0}) &&J^{(1(\frac12\frac12))}_{0-\frac12\frac12} = \tfrac{1}{\sqrt3}(\sqrt2 i J^{H}_{-1} - J^{G}_{-1})\\
&J^{(1(\frac12\frac12))}_{-1-\frac12\frac12} = \tfrac{1}{2\sqrt3}(-i J^{H}_{-2} - 2\sqrt2 J^{G}_{-2} + \sqrt3 J^{T_2}_{-2}) &&J^{(1(\frac12\frac12))}_{1-\frac12-\frac12} = \tfrac{1}{\sqrt3}(\sqrt2 J^{G}_{-1} + i J^{H}_{-1})\\
&J^{(1(\frac12\frac12))}_{0-\frac12-\frac12} = \tfrac{1}{\sqrt6}(-\sqrt3 J^{T_2}_{-2} - \sqrt2 J^{G}_{-2} + i J^{H}_{-2}) &&J^{(1(\frac12\frac12))}_{-1-\frac12-\frac12} = \tfrac12(J^{T_2}_{2} - \sqrt3 i J^{H}_{2})
\end{aligned} \tag{86}$$

where the notation $J^{\Lambda}_{i} = (\Lambda i(G, T_1))$ is adopted for brevity.

A.3.3. (T_2, G). The embedding of the icosahedral operators T_1, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is as follows:

$$J^{(1(\frac12\frac12))}_{1\frac12\frac12} = \frac{1}{\sqrt2}(J^H_0 - iJ^{T_1}_0) \qquad J^{(1(\frac12\frac12))}_{0\frac12\frac12} = \frac{1}{\sqrt3}(iJ^G_2 - \sqrt2 J^H_2)$$
$$J^{(1(\frac12\frac12))}_{-1\frac12\frac12} = \frac{1}{2\sqrt3}(\sqrt3 iJ^{T_1}_{-1} + 2\sqrt2 iJ^G_{-1} - J^H_{-1}) \qquad J^{(1(\frac12\frac12))}_{1\frac12-\frac12} = \frac12(iJ^{T_1}_{-1} + \sqrt3 J^H_{-1})$$
$$J^{(1(\frac12\frac12))}_{0\frac12-\frac12} = \frac{1}{\sqrt6}(\sqrt3 iJ^{T_1}_1 - \sqrt2 iJ^G_1 + J^H_1) \qquad J^{(1(\frac12\frac12))}_{-1\frac12-\frac12} = \frac{1}{\sqrt3}(\sqrt2 iJ^G_{-2} - J^H_{-2})$$
$$J^{(1(\frac12\frac12))}_{1-\frac12\frac12} = \frac{1}{\sqrt3}(\sqrt2 iJ^G_2 + J^H_2) \qquad J^{(1(\frac12\frac12))}_{0-\frac12\frac12} = \frac{1}{\sqrt6}(-\sqrt3 iJ^{T_1}_{-1} + \sqrt2 iJ^G_{-1} + J^H_{-1})$$
$$J^{(1(\frac12\frac12))}_{-1-\frac12\frac12} = \frac12(iJ^{T_1}_1 - \sqrt3 J^H_1) \qquad J^{(1(\frac12\frac12))}_{1-\frac12-\frac12} = \frac{1}{2\sqrt3}(-\sqrt3 iJ^{T_1}_1 - 2\sqrt2 iJ^G_1 - J^H_1)$$
$$J^{(1(\frac12\frac12))}_{0-\frac12-\frac12} = \frac{1}{\sqrt3}(iJ^G_{-2} + \sqrt2 J^H_{-2}) \qquad J^{(1(\frac12\frac12))}_{-1-\frac12-\frac12} = \frac{1}{\sqrt2}(iJ^{T_1}_0 + J^H_0) \tag{87}$$

where the notation $J^\Lambda_i = (\Lambda i(T_2, G))$ is adopted for brevity.

A.3.4. (G, T_2). The embedding of the icosahedral operators T_1, G and H in the irrep $(1(\frac{1}{2}\frac{1}{2}))$ is as follows:

$$J^{(1(\frac12\frac12))}_{1\frac12\frac12} = \frac{1}{\sqrt2}(iJ^{T_1}_0 + J^H_0) \qquad J^{(1(\frac12\frac12))}_{0\frac12\frac12} = \frac{1}{\sqrt3}(iJ^G_2 - \sqrt2 J^H_2)$$
$$J^{(1(\frac12\frac12))}_{-1\frac12\frac12} = \frac{1}{2\sqrt3}(-i\sqrt3 J^{T_1}_{-1} + i2\sqrt2 J^G_{-1} - J^H_{-1}) \qquad J^{(1(\frac12\frac12))}_{1\frac12-\frac12} = \frac12(-iJ^{T_1}_{-1} + \sqrt3 J^H_{-1})$$
$$J^{(1(\frac12\frac12))}_{0\frac12-\frac12} = \frac{1}{\sqrt6}(-\sqrt3 iJ^{T_1}_1 - \sqrt2 iJ^G_1 + J^H_1) \qquad J^{(1(\frac12\frac12))}_{-1\frac12-\frac12} = \frac{1}{\sqrt3}(\sqrt2 iJ^G_{-2} - J^H_{-2})$$
$$J^{(1(\frac12\frac12))}_{1-\frac12\frac12} = \frac{1}{\sqrt3}(\sqrt2 iJ^G_2 + J^H_2) \qquad J^{(1(\frac12\frac12))}_{0-\frac12\frac12} = \frac{1}{\sqrt6}(\sqrt3 iJ^{T_1}_{-1} + \sqrt2 iJ^G_{-1} + J^H_{-1})$$
$$J^{(1(\frac12\frac12))}_{-1-\frac12\frac12} = \frac12(-iJ^{T_1}_1 - \sqrt3 J^H_1) \qquad J^{(1(\frac12\frac12))}_{1-\frac12-\frac12} = \frac{1}{2\sqrt3}(\sqrt3 iJ^{T_1}_1 - 2\sqrt2 iJ^G_1 - J^H_1)$$
$$J^{(1(\frac12\frac12))}_{0-\frac12-\frac12} = \frac{1}{\sqrt3}(iJ^G_{-2} + \sqrt2 J^H_{-2}) \qquad J^{(1(\frac12\frac12))}_{-1-\frac12-\frac12} = \frac{1}{\sqrt2}(-iJ^{T_1}_0 + J^H_0) \tag{88}$$

where the notation $J^\Lambda_i = (\Lambda i(G, T_2))$ is adopted for brevity.

A.4. Embedding of the (T_1, H), (H, T_1), (T_2, H) and (H, T_2) icosahedral operators

A.4.1. (T_1, H). The embedding of the icosahedral operators T_1, T_2, G and H in the irrep $(1[10])$ is as follows:

$$J^{(1[10])}_{110} = \frac{1}{\sqrt5}(-\sqrt2 iJ^{T_2}_{-2} + \sqrt3 iJ^G_{-2}) \qquad J^{(1[10])}_{101} = \frac{1}{\sqrt{15}}(-\sqrt6 iJ^{T_2}_2 - 2iJ^G_2 + \sqrt5 J^H_2)$$
$$J^{(1[10])}_{100} = \frac{1}{\sqrt{10}}(-iJ^{T_1}_1 + 2iJ^G_1 + \sqrt5 J^H_1) \qquad J^{(1[10])}_{10-1} = \frac{1}{\sqrt{10}}(-\sqrt3 iJ^{T_1}_0 - \sqrt2 iJ^{T_2}_0 + \sqrt5 J^H_0)$$
$$J^{(1[10])}_{1-10} = \frac{1}{\sqrt{15}}(3iJ^{T_1}_{-1} - iJ^G_{-1} - \sqrt5 J^H_{-1}) \qquad J^{(1[10])}_{010} = \frac{1}{\sqrt{15}}(\sqrt3 iJ^{T_2}_2 + \sqrt2 iJ^G_2 + \sqrt{10} J^H_2)$$
$$J^{(1[10])}_{001} = \frac{1}{\sqrt{30}}(3iJ^{T_1}_1 + 4iJ^G_1 - \sqrt5 J^H_1) \qquad J^{(1[10])}_{000} = \frac{1}{\sqrt5}(-\sqrt2 iJ^{T_1}_0 + \sqrt3 iJ^{T_2}_0)$$
$$J^{(1[10])}_{00-1} = \frac{1}{\sqrt{30}}(-3iJ^{T_1}_{-1} - 4iJ^G_{-1} - \sqrt5 J^H_{-1}) \qquad J^{(1[10])}_{0-10} = \frac{1}{\sqrt{15}}(\sqrt3 iJ^{T_2}_{-2} + \sqrt2 iJ^G_{-2} - \sqrt{10} J^H_{-2})$$
$$J^{(1[10])}_{-110} = \frac{1}{\sqrt{15}}(-3iJ^{T_1}_1 + iJ^G_1 - \sqrt5 J^H_1) \qquad J^{(1[10])}_{-101} = \frac{1}{\sqrt{10}}(-\sqrt3 iJ^{T_1}_0 - \sqrt2 iJ^{T_2}_0 - \sqrt5 J^H_0)$$
$$J^{(1[10])}_{-100} = \frac{1}{\sqrt{10}}(iJ^{T_1}_{-1} - 2iJ^G_{-1} + \sqrt5 J^H_{-1}) \qquad J^{(1[10])}_{-10-1} = \frac{1}{\sqrt{15}}(-\sqrt6 iJ^{T_2}_{-2} - 2iJ^G_{-2} - \sqrt5 J^H_{-2})$$
$$J^{(1[10])}_{-1-10} = \frac{1}{\sqrt5}(\sqrt2 iJ^{T_2}_2 - \sqrt3 iJ^G_2) \tag{89}$$

where the notation $J_i^{\Lambda} = (\Lambda i(T_1, H))$ is adopted for brevity.

A.4.2. (H, T_1). The embedding of the icosahedral operators T_1, T_2, G and H in the irrep (1[10]) is as follows:

$$
\begin{aligned}
&J_{110}^{(1[10])} = \tfrac{1}{\sqrt{5}}(-\sqrt{2}i J_{-2}^{T_2} - \sqrt{3}i J_{-2}^{G}) \qquad J_{101}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{6}i J_{2}^{T_2} + 2i J_{2}^{G} - \sqrt{5}J_{2}^{H})\\
&J_{100}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-i J_{1}^{T_1} - 2i J_{1}^{G} - \sqrt{5}J_{1}^{H}) \qquad J_{10-1}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-\sqrt{3}i J_{0}^{T_1} - \sqrt{2}i J_{0}^{T_2} - \sqrt{5}J_{0}^{H})\\
&J_{1-10}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-3i J_{-1}^{T_1} - i J_{-1}^{G} - \sqrt{5}J_{-1}^{H}) \qquad J_{010}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{3}i J_{2}^{T_2} - \sqrt{2}i J_{2}^{G} - \sqrt{10}J_{2}^{H})\\
&J_{001}^{(1[10])} = \tfrac{1}{\sqrt{30}}(3i J_{1}^{T_1} - 4i J_{1}^{G} + \sqrt{5}J_{1}^{H}) \qquad J_{000}^{(1[10])} = \tfrac{1}{\sqrt{5}}(\sqrt{2}i J_{0}^{T_1} - \sqrt{3}i J_{0}^{T_2})\\
&J_{00-1}^{(1[10])} = \tfrac{1}{\sqrt{30}}(-3i J_{-1}^{T_1} + 4i J_{-1}^{G} + \sqrt{5}J_{-1}^{H}) \qquad J_{0-10}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{3}i J_{-2}^{T_2} - \sqrt{2}i J_{-2}^{G} + \sqrt{10}J_{-2}^{H})\\
&J_{-110}^{(1[10])} = \tfrac{1}{\sqrt{15}}(3i J_{1}^{T_1} + i J_{1}^{G} - \sqrt{5}J_{1}^{H}) \qquad J_{-101}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-\sqrt{3}i J_{0}^{T_1} - \sqrt{2}i J_{0}^{T_2} + \sqrt{5}J_{0}^{H})\\
&J_{-100}^{(1[10])} = \tfrac{1}{\sqrt{10}}(i J_{-1}^{T_1} + 2i J_{-1}^{G} - \sqrt{5}J_{-1}^{H}) \qquad J_{-10-1}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{6}i J_{-2}^{T_2} + 2i J_{-2}^{G} + \sqrt{5}J_{-2}^{H})\\
&J_{-1-10}^{(1[10])} = \tfrac{1}{\sqrt{5}}(\sqrt{2}i J_{2}^{T_2} + \sqrt{3}i J_{2}^{G})
\end{aligned}
\tag{90}
$$

where the notation $J_i^{\Lambda} = (\Lambda i(H, T_1))$ is adopted for brevity.

A.4.3. (T_2, H). The embedding of the icosahedral operators T_1, T_2, G and H in the irrep (1[10]) is as follows:

$$
\begin{aligned}
&J_{110}^{(1[10])} = \tfrac{1}{\sqrt{10}}(\sqrt{2}i J_{0}^{T_1} + \sqrt{3}i J_{0}^{T_2} + \sqrt{5}J_{0}^{H}) \qquad J_{101}^{(1[10])} = \tfrac{1}{\sqrt{5}}(\sqrt{2}i J_{-1}^{T_1} + \sqrt{3}i J_{-1}^{G})\\
&J_{100}^{(1[10])} = \tfrac{1}{\sqrt{10}}(i J_{-2}^{T_2} - 2i J_{-2}^{G} - \sqrt{5}J_{-2}^{H}) \qquad J_{10-1}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-3i J_{2}^{T_2} + i J_{2}^{G} + \sqrt{5}J_{2}^{H})\\
&J_{1-10}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{6}i J_{1}^{T_1} - 2i J_{1}^{G} - \sqrt{5}J_{1}^{H}) \qquad J_{010}^{(1[10])} = \tfrac{1}{\sqrt{30}}(-3i J_{2}^{T_2} - 4i J_{2}^{G} - \sqrt{5}J_{2}^{H})\\
&J_{001}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{3}i J_{1}^{T_1} + \sqrt{2}i J_{1}^{G} - \sqrt{10}J_{1}^{H}) \qquad J_{000}^{(1[10])} = \tfrac{1}{\sqrt{5}}(\sqrt{3}i J_{0}^{T_1} - \sqrt{2}i J_{0}^{T_2})\\
&J_{00-1}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{3}i J_{-1}^{T_1} - \sqrt{2}i J_{-1}^{G} - \sqrt{10}J_{-1}^{H}) \qquad J_{0-10}^{(1[10])} = \tfrac{1}{\sqrt{30}}(-3i J_{-2}^{T_2} - 4i J_{-2}^{G} + \sqrt{5}J_{-2}^{H})\\
&J_{-110}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{6}i J_{-1}^{T_1} + 2i J_{-1}^{G} - \sqrt{5}J_{-1}^{H}) \qquad J_{-101}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-3i J_{-2}^{T_2} + i J_{-2}^{G} - \sqrt{5}J_{-2}^{H})\\
&J_{-100}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-i J_{2}^{T_2} + 2i J_{2}^{G} - \sqrt{5}J_{2}^{H}) \qquad J_{-10-1}^{(1[10])} = \tfrac{1}{\sqrt{5}}(\sqrt{2}i J_{1}^{T_1} + \sqrt{3}i J_{1}^{G})\\
&J_{-1-10}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-\sqrt{2}i J_{0}^{T_1} - \sqrt{3}i J_{0}^{T_2} + \sqrt{5}J_{0}^{H})
\end{aligned}
\tag{91}
$$

where the notation $J_i^{\Lambda} = (\Lambda i(T_2, H))$ is adopted for brevity.

A.4.4 (H, T_2). The embedding of the icosahedral operators T_1, T_2, G and H in the irrep (1[10]) is as follows:

$$
\begin{aligned}
&J_{110}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-\sqrt{2}i J_{0}^{T_1} - \sqrt{3}i J_{0}^{T_2} + \sqrt{5}J_{0}^{H}) \qquad J_{101}^{(1[10])} = \tfrac{1}{\sqrt{5}}(-\sqrt{2}i J_{-1}^{T_1} + \sqrt{3}i J_{-1}^{G})\\
&J_{100}^{(1[10])} = \tfrac{1}{\sqrt{10}}(-i J_{-2}^{T_2} - 2i J_{-2}^{G} - \sqrt{5}J_{-2}^{H}) \qquad J_{10-1}^{(1[10])} = \tfrac{1}{\sqrt{15}}(3i J_{2}^{T_2} + i J_{2}^{G} + \sqrt{5}J_{2}^{H})\\
&J_{1-10}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{6}i J_{1}^{T_1} - 2i J_{1}^{G} - \sqrt{5}J_{1}^{H}) \qquad J_{010}^{(1[10])} = \tfrac{1}{\sqrt{30}}(3i J_{2}^{T_2} - 4i J_{2}^{G} - \sqrt{5}J_{2}^{H})\\
&J_{001}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{3}i J_{1}^{T_1} + \sqrt{2}i J_{1}^{G} - \sqrt{10}J_{1}^{H}) \qquad J_{000}^{(1[10])} = \tfrac{1}{\sqrt{5}}(-\sqrt{3}i J_{0}^{T_1} + \sqrt{2}i J_{0}^{T_2})\\
&J_{00-1}^{(1[10])} = \tfrac{1}{\sqrt{15}}(-\sqrt{3}i J_{-1}^{T_1} - \sqrt{2}i J_{-1}^{G} - \sqrt{10}J_{-1}^{H}) \qquad J_{0-10}^{(1[10])} = \tfrac{1}{\sqrt{30}}(3i J_{-2}^{T_2} - 4i J_{-2}^{G} + \sqrt{5}J_{-2}^{H})\\
&J_{-110}^{(1[10])} = \tfrac{1}{\sqrt{15}}(\sqrt{6}i J_{-1}^{T_1} + 2i J_{-1}^{G} - \sqrt{5}J_{-1}^{H}) \qquad J_{-101}^{(1[10])} = \tfrac{1}{\sqrt{15}}(3i J_{-2}^{T_2} + i J_{-2}^{G} - \sqrt{5}J_{-2}^{H})
\end{aligned}
$$

$$J^{(1[10])}_{-100} = \frac{1}{\sqrt{10}}(iJ^{T_2}_2 + 2iJ^G_2 - \sqrt{5}J^H_2) \qquad J^{(1[10])}_{-10-1} = \frac{1}{\sqrt{5}}(-\sqrt{2}iJ^{T_1}_1 + \sqrt{3}iJ^G_1)$$
$$J^{(1[10])}_{-1-10} = \frac{1}{\sqrt{10}}(\sqrt{2}iJ^{T_1}_0 + \sqrt{3}iJ^{T_2}_0 + \sqrt{5}J^H_0) \tag{92}$$

where the notation $J^{\Lambda}_i = (\Lambda i(H, T_2))$ is adopted for brevity.

A.5. Embedding of the (G, H) and (H, G) icosahedral operators

A.5.1. (G, H). The embedding of the icosahedral operators T_1, T_2, G, ${}^1H$ and ${}^2H$ in the irrep $((\frac{1}{2}\frac{1}{2})[10])$ is as follows:

$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}10} = \frac{1}{2\sqrt{30}}(3\sqrt{6}J^{T_1}_{-1} + 4J^G_{-1} + 3\sqrt{5}iJ^{{}^1H}_{-1} - \sqrt{5}iJ^{{}^2H}_{-1})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}01} = \frac{1}{2\sqrt{30}}(-\sqrt{6}J^{T_2}_{-2} + 8J^G_{-2} - 3\sqrt{5}iJ^{{}^1H}_{-2} - \sqrt{5}iJ^{{}^2H}_{-2})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}00} = \frac{1}{2\sqrt{10}}(-2\sqrt{3}J^{T_2}_2 - 2\sqrt{2}J^G_2 + \sqrt{10}iJ^{{}^1H}_2 - \sqrt{10}iJ^{{}^2H}_2)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}0-1} = \frac{1}{\sqrt{15}}(\sqrt{3}J^{T_1}_1 - \sqrt{2}J^G_1 - \sqrt{10}iJ^{{}^2H}_1)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}-10} = \frac{1}{2\sqrt{10}}(-2J^{T_1}_0 - 4J^{T_2}_0 + \sqrt{10}iJ^{{}^1H}_0 + \sqrt{10}iJ^{{}^2H}_0)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}10} = \frac{1}{\sqrt{15}}(-\sqrt{3}J^{T_2}_{-2} - \sqrt{2}J^G_{-2} - \sqrt{10}iJ^{{}^2H}_{-2})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}01} = \frac{1}{2\sqrt{30}}(-3\sqrt{6}J^{T_2}_2 + 4J^G_2 - 3\sqrt{5}iJ^{{}^1H}_2 - \sqrt{5}iJ^{{}^2H}_2)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}00} = \frac{1}{2\sqrt{5}}(-\sqrt{6}J^{T_1}_1 + 2J^G_1 - \sqrt{5}iJ^{{}^1H}_1 - \sqrt{5}iJ^{{}^2H}_1)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}0-1} = \frac{1}{2\sqrt{5}}(-2\sqrt{2}J^{T_1}_0 + \sqrt{2}J^{T_2}_0 + \sqrt{5}iJ^{{}^1H}_0 - \sqrt{5}iJ^{{}^2H}_0)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}-10} = \frac{1}{2\sqrt{30}}(\sqrt{6}J^{T_1}_{-1} + 8J^G_{-1} - 3\sqrt{5}iJ^{{}^1H}_{-1} + \sqrt{5}iJ^{{}^2H}_{-1})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}10} = \frac{1}{2\sqrt{30}}(-\sqrt{6}J^{T_1}_1 - 8J^G_1 - 3\sqrt{5}iJ^{{}^1H}_1 + \sqrt{5}iJ^{{}^2H}_1)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}01} = \frac{1}{2\sqrt{5}}(-2\sqrt{2}J^{T_1}_0 + \sqrt{2}J^{T_2}_0 - \sqrt{5}iJ^{{}^1H}_0 + \sqrt{5}iJ^{{}^2H}_0)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}00} = \frac{1}{2\sqrt{5}}(\sqrt{6}J^{T_1}_{-1} - 2J^G_{-1} - \sqrt{5}iJ^{{}^1H}_{-1} - \sqrt{5}iJ^{{}^2H}_{-1})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}0-1} = \frac{1}{2\sqrt{30}}(-3\sqrt{6}J^{T_2}_{-2} + 4J^G_{-2} + 3\sqrt{5}iJ^{{}^1H}_{-2} + \sqrt{5}iJ^{{}^2H}_{-2})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}-10} = \frac{1}{\sqrt{15}}(\sqrt{3}J^{T_2}_2 + \sqrt{2}J^G_2 - \sqrt{10}iJ^{{}^2H}_2)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}10} = \frac{1}{2\sqrt{10}}(-2J^{T_1}_0 - 4J^{T_2}_0 - \sqrt{10}iJ^{{}^1H}_0 - \sqrt{10}iJ^{{}^2H}_0)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}01} = \frac{1}{\sqrt{15}}(-\sqrt{3}J^{T_1}_{-1} + \sqrt{2}J^G_{-1} - \sqrt{10}iJ^{{}^2H}_{-1})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}00} = \frac{1}{2\sqrt{10}}(-2\sqrt{3}J^{T_2}_{-2} - 2\sqrt{2}J^G_{-2} - \sqrt{10}iJ^{{}^1H}_{-2} + \sqrt{10}iJ^{{}^2H}_{-2})$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}0-1} = \frac{1}{2\sqrt{30}}(\sqrt{6}J^{T_2}_2 - 8J^G_2 - 3\sqrt{5}iJ^{{}^1H}_2 - \sqrt{5}iJ^{{}^2H}_2)$$
$$J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}-10} = \frac{1}{2\sqrt{30}}(3\sqrt{6}J^{T_1}_1 + 4J^G_1 - 3\sqrt{5}iJ^{{}^1H}_1 + \sqrt{5}iJ^{{}^2H}_1) \tag{93}$$

where the notation $J^{\Lambda}_i = (\Lambda i(G, H))$ is adopted for brevity.

A.5.2. (H, G). The embedding of the icosahedral operators T_1, T_2, G, ${}^1H$ and ${}^2H$ in the irrep $((\frac{1}{2}\frac{1}{2})[10])$ is as follows:

$$
\begin{aligned}
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}10} &= \tfrac{1}{2\sqrt{30}}(3\sqrt{6}iJ^{T_1}_{-1} - 4iJ^{G}_{-1} - 3\sqrt{5}J^{^1H}_{-1} - \sqrt{5}J^{^2H}_{-1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}01} &= \tfrac{1}{2\sqrt{30}}(\sqrt{6}iJ^{T_2}_{-2} + 8iJ^{G}_{-2} - 3\sqrt{5}J^{^1H}_{-2} + \sqrt{5}J^{^2H}_{-2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}00} &= \tfrac{1}{2\sqrt{5}}(\sqrt{6}iJ^{T_2}_{2} - 2iJ^{G}_{2} + \sqrt{5}J^{^1H}_{2} + \sqrt{5}J^{^2H}_{2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}0-1} &= \tfrac{1}{\sqrt{30}}(\sqrt{6}iJ^{T_1}_{1} + 2iJ^{G}_{1} - 2\sqrt{5}J^{^2H}_{1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}\frac{1}{2}-10} &= \tfrac{1}{2\sqrt{5}}(-\sqrt{2}iJ^{T_1}_{0} - 2\sqrt{2}iJ^{T_2}_{0} - \sqrt{5}J^{^1H}_{0} + \sqrt{5}J^{^2H}_{0})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}10} &= \tfrac{1}{\sqrt{30}}(\sqrt{6}iJ^{T_2}_{-2} + 2iJ^{G}_{-2} - 2\sqrt{5}J^{^2H}_{-2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}01} &= \tfrac{1}{2\sqrt{30}}(3\sqrt{6}iJ^{T_2}_{2} + 4iJ^{G}_{2} - 3\sqrt{5}J^{^1H}_{2} + \sqrt{5}J^{^2H}_{2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}00} &= \tfrac{1}{2\sqrt{5}}(-\sqrt{6}iJ^{T_1}_{1} - 2iJ^{G}_{1} + \sqrt{5}J^{^1H}_{1} - \sqrt{5}J^{^2H}_{1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}0-1} &= \tfrac{1}{2\sqrt{5}}(2\sqrt{2}iJ^{T_1}_{0} - \sqrt{2}iJ^{T_2}_{0} + \sqrt{5}J^{^1H}_{0} + \sqrt{5}J^{^2H}_{0})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{\frac{1}{2}-\frac{1}{2}-10} &= \tfrac{1}{2\sqrt{30}}(\sqrt{6}iJ^{T_1}_{-1} - 8iJ^{G}_{-1} + 3\sqrt{5}J^{^1H}_{-1} + \sqrt{5}J^{^2H}_{-1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}10} &= \tfrac{1}{2\sqrt{30}}(\sqrt{6}iJ^{T_1}_{1} - 8iJ^{G}_{1} - 3\sqrt{5}J^{^1H}_{1} - \sqrt{5}J^{^2H}_{1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}01} &= \tfrac{1}{2\sqrt{5}}(-2\sqrt{2}iJ^{T_1}_{0} + \sqrt{2}iJ^{T_2}_{0} + \sqrt{5}J^{^1H}_{0} + \sqrt{5}J^{^2H}_{0})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}00} &= \tfrac{1}{2\sqrt{5}}(-\sqrt{6}iJ^{T_1}_{-1} - 2iJ^{G}_{-1} - \sqrt{5}J^{^1H}_{-1} + \sqrt{5}J^{^2H}_{-1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}0-1} &= \tfrac{1}{2\sqrt{30}}(-3\sqrt{6}iJ^{T_2}_{-2} - 4iJ^{G}_{-2} - 3\sqrt{5}J^{^1H}_{-2} + \sqrt{5}J^{^2H}_{-2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}\frac{1}{2}-10} &= \tfrac{1}{\sqrt{30}}(\sqrt{6}iJ^{T_2}_{2} - 2iJ^{G}_{2} - 2\sqrt{5}J^{^2H}_{2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}10} &= \tfrac{1}{2\sqrt{5}}(\sqrt{2}iJ^{T_1}_{0} + 2\sqrt{2}iJ^{T_2}_{0} - \sqrt{5}J^{^1H}_{0} + \sqrt{5}J^{^2H}_{0})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}01} &= \tfrac{1}{\sqrt{30}}(\sqrt{6}iJ^{T_1}_{-1} + 2iJ^{G}_{-1} + 2\sqrt{5}J^{^2H}_{-1})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}00} &= \tfrac{1}{2\sqrt{5}}(-\sqrt{6}iJ^{T_2}_{-2} + 2iJ^{G}_{-2} + \sqrt{5}J^{^1H}_{-2} + \sqrt{5}J^{^2H}_{-2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}0-1} &= \tfrac{1}{2\sqrt{30}}(\sqrt{6}iJ^{T_2}_{2} + 8iJ^{G}_{2} + 3\sqrt{5}J^{^1H}_{2} - \sqrt{5}J^{^2H}_{2})\\
J^{((\frac{1}{2}\frac{1}{2})[10])}_{-\frac{1}{2}-\frac{1}{2}-10} &= \tfrac{1}{2\sqrt{30}}(-3\sqrt{6}iJ^{T_1}_{1} + 4iJ^{G}_{1} - 3\sqrt{5}J^{^1H}_{1} - \sqrt{5}J^{^2H}_{1})
\end{aligned}
\tag{94}
$$

where the notation $J^{\Lambda}_{i} = (\Lambda i(H, G))$ is adopted for brevity.

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