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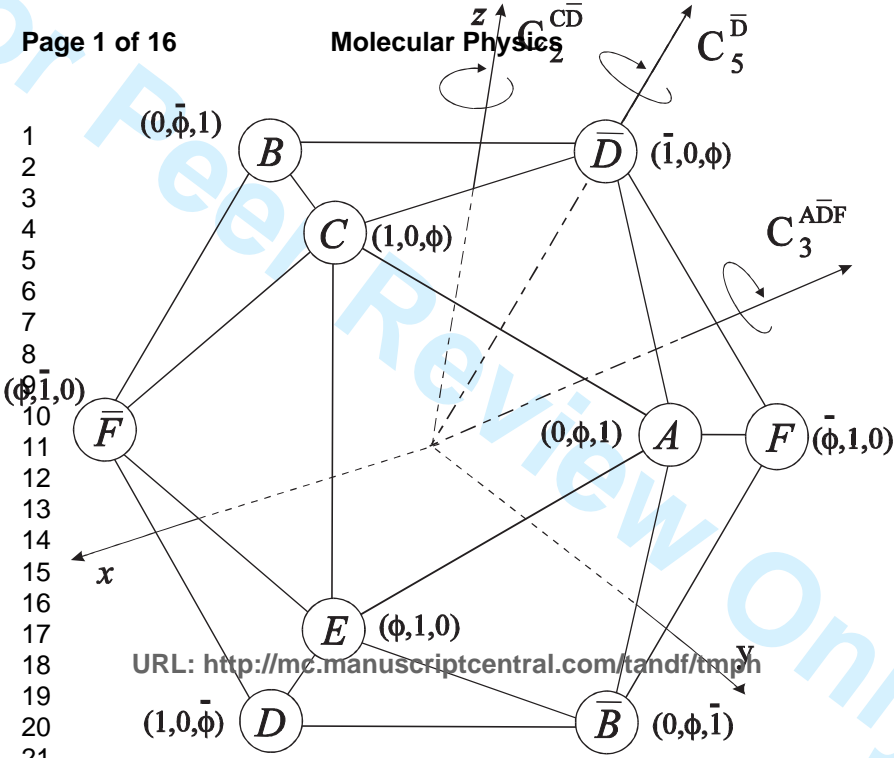
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JTConstruct.tex	



Construction of the $\Gamma_9 \times (g + 2h)$ Jahn-Teller Hamiltonian

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The coupling coefficients describing the linear $\Gamma_9 \times (g + 2h)$ Jahn-Teller Hamiltonian in icosahedral symmetry are derived, and various coupling schemes are discussed.

1 Introduction

The highest degeneracy that a finite point group can sustain is sixfold and corresponds to the Γ_9 irreducible representation (irrep) in the icosahedral double group, I^* . In a recent work we have presented for the first time the solutions to the corresponding Jahn-Teller (JT) Hamiltonian [1]. At present we provide a detailed derivation of the coupling coefficients that are needed to construct this Hamiltonian. The derivation is based on our 1993 paper [2], presenting the spin-orbit coupling tables for the icosahedral double group. The active modes are obtained from the antisymmetric direct product of the spin representation, less the totally symmetric irrep:

$$\{\Gamma_9 \times \Gamma_9\} - A_1 = G + 2H, \quad (1)$$

giving rise to the $\Gamma_9 \times (g + 2h)$ Hamiltonian [3]. Only linear Jahn-Teller forces will be considered. In addition the Hamiltonian is bound by the harmonic restoring forces which provide a totally symmetric background.

2 The orbital and spin basis

Our work is based on the real orbital basis introduced by Boyle and Parker [4]. This basis follows a $I \downarrow D_2$ subduction scheme, where the Cartesian coordinates are oriented along three twofold axes of the icosahedron [5], as indicated in Figure 1. The component labeling of the orbital representations is shown in Table 1. It should be noted that $H\theta$ and $H\epsilon$ are linear combinations of the canonical $H(d_{z^2})$ and $H(d_{x^2-y^2})$

Table 1. Icosahedral orbital representations: labeling of the real components

Representation	Components
A	$ Aa\rangle$
T_1	$ T_1x\rangle, T_1y\rangle, T_1z\rangle$
T_2	$ T_2x\rangle, T_2y\rangle, T_2z\rangle$
G	$ Ga\rangle, Gx\rangle, Gy\rangle, Gz\rangle$
H	$ H\theta\rangle, H\epsilon\rangle, Hx\rangle, Hy\rangle, Hz\rangle$

Table 2. Icosahedral orbital representations: complex components

Representation	Components
A	$ Aa\rangle$
T_1	$ T_11\rangle = -\frac{1}{\sqrt{2}}(T_1x\rangle + i T_1y\rangle)$ $ T_1-1\rangle = \frac{1}{\sqrt{2}}(T_1x\rangle - i T_1y\rangle)$ $ T_10\rangle = T_1z\rangle$
T_2	$ T_21\rangle = -\frac{1}{\sqrt{2}}(T_2x\rangle + i T_2y\rangle)$ $ T_2-1\rangle = \frac{1}{\sqrt{2}}(T_2x\rangle - i T_2y\rangle)$ $ T_20\rangle = T_2z\rangle$
G	$ Gi\rangle = i Ga\rangle$ $ G1\rangle = -\frac{1}{\sqrt{2}}(Gx\rangle + i Gy\rangle)$ $ G-1\rangle = \frac{1}{\sqrt{2}}(Gx\rangle - i Gy\rangle)$ $ G0\rangle = Gz\rangle$
H	$ H2\rangle = \frac{1}{4}(\sqrt{5} H\theta\rangle + \sqrt{3} H\epsilon\rangle + i\sqrt{8} Hz\rangle)$ $ H-2\rangle = \frac{1}{4}(\sqrt{5} H\theta\rangle + \sqrt{3} H\epsilon\rangle - i\sqrt{8} Hz\rangle)$ $ H1\rangle = -\frac{1}{\sqrt{2}}(i Hx\rangle + Hy\rangle)$ $ H-1\rangle = -\frac{1}{\sqrt{2}}(i Hx\rangle - Hy\rangle)$ $ H0\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3} H\theta\rangle - \sqrt{5} H\epsilon\rangle)$

components:

$$\begin{aligned}
 H\theta &= \sqrt{\frac{3}{8}}H(d_{z^2}) + \sqrt{\frac{5}{8}}H(d_{x^2-y^2}) \\
 H\epsilon &= -\sqrt{\frac{5}{8}}H(d_{z^2}) + \sqrt{\frac{3}{8}}H(d_{x^2-y^2})
 \end{aligned} \tag{2}$$

For the construction of spin-orbit coupling coefficients we have transformed this basis into complex form (see Table 2). The choice of the complex components is based on the requirement that there be a *conjugating element*, R_0 , that turns the components into partners with complex conjugate transformation properties [2]. Hence R_0 triggers an inner automorphism $R \rightarrow R_0^{-1}RR_0$ that takes the representational

matrices, $\mathbf{D}^\Gamma(R)$, of a given irrep Γ into their complex conjugates, i.e.:

$$\mathbf{D}^\Gamma(R_0^{-1}RR_0) = \overline{\mathbf{D}^\Gamma(R)} \quad (3)$$

Following the Wigner-Racah convention for spherical symmetry, the C_2^y axis along the y -direction is chosen as the conjugating element. The fivefold degenerate H representation is the descendant of the spherical $J = 2$ quadrupole representation, and its complex components were chosen in accordance with the conventional Racah conjugation relationship:

$$C_2^y|JM\rangle = (-1)^{J-M}|J-M\rangle \quad (4)$$

This $|JM\rangle$ basis is connected to the real basis of Boyle and Parker as indicated in Table 2. We will arrange these complex H components in a row vector:

$$|\mathbf{H}\rangle = (|H2\rangle |H-2\rangle |H1\rangle |H-1\rangle |H0\rangle) \quad (5)$$

The action of the conjugating element, R_0 , is thus given by:

$$C_2^y|\mathbf{H}\rangle = |\mathbf{H}\rangle \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (6)$$

The choice of complex components for the G -basis is less straightforward since there is no fourfold degenerate parent spherical representation. We have transformed the x, y, z components of G into a complex form using the standard conventions for the Cartesian basis set, exactly as described by the T_1 orbital basis. The inner automorphism can then be satisfied by requiring that the remaining fourth component $|Ga\rangle$ be multiplied by the imaginary. The phase-adapted component is denoted as $|Gi\rangle$. The resulting expressions are shown in Table 2.

We arrange the complex G -components in a row vector as:

$$|\mathbf{G}\rangle = (|Gi\rangle |G1\rangle |G-1\rangle |G0\rangle) \quad (7)$$

The action of the conjugated element on the complex G -basis is then:

$$C_2^y|\mathbf{G}\rangle = |\mathbf{G}\rangle \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (8)$$

Finally the $J = 5/2$ spherical spin basis subduces at once the icosahedral Γ_9 irrep, so that the six components may be labeled by spherical M -labels, as:

$$|\mathbf{\Gamma}_9\rangle = (|+\frac{5}{2}\rangle |+\frac{3}{2}\rangle |+\frac{1}{2}\rangle |-\frac{1}{2}\rangle |-\frac{3}{2}\rangle |-\frac{5}{2}\rangle) \quad (9)$$

This basis obeys the standard Racah conjugation, as described in (4). Its transformation properties under the group generators were given earlier [2].

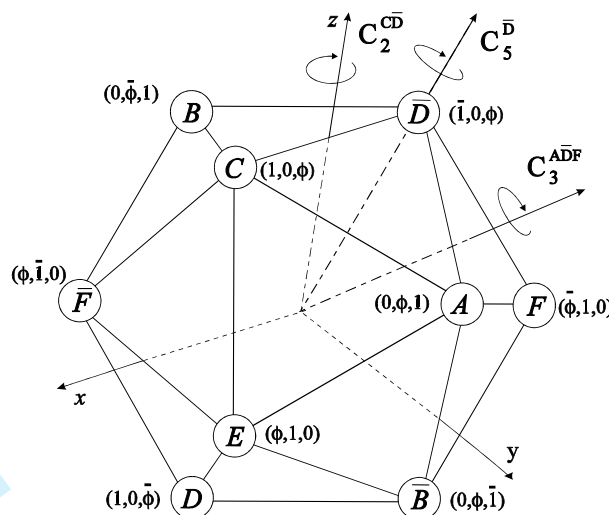


Figure 1. The icosahedron showing the co-ordinates of the vertices and axes of rotation (ϕ is the golden number and the overbar denotes the minus sign or inversion)

3 Time reversal

In the present problem, time reversal plays a very important role since the Jahn-Teller distortions are time even and cannot break time reversal symmetry. The time reversal operator is an antilinear operator. It consists of two parts: complex conjugation of all scalar coefficients and reversal of any ket-function into a ket-function for which time runs oppositely [6]. The time-reversed component of a given ket $|\Gamma\gamma\rangle$ is indicated by a star, and can be obtained from our automorphism operator R_0 :

$$|\Gamma\gamma^*\rangle \equiv R_0|\Gamma\gamma\rangle \tag{10}$$

The corresponding bras are formed by inverting this equation:

$$\langle\Gamma\gamma^*| = \langle\Gamma\gamma|R_0^{-1} \tag{11}$$

Applying the star operator twice leads to the identity operator in the case of orbital representations and minus the identity for spin representations, which is precisely the criterion for time reversal. Since the orbital representations can also be expressed as linear combinations of real functions (see Table 2), the action of R_0 and complex conjugation on these components can directly be compared. One verifies that for the H-representations, complex conjugation and R_0 coincide, while for the complex G-components the present choice of complex components involves a sign difference between the two operations, i.e.:

$$\begin{aligned} \forall\gamma \in G : |G\gamma^*\rangle &= -|\overline{G\gamma}\rangle \\ \forall\eta \in H : |H\eta^*\rangle &= |\overline{H\eta}\rangle, \end{aligned} \tag{12}$$

where the overbar denotes complex conjugation. The sign change for G is a result of the choice of complex components. It could be absorbed by multiplying the basis with i . However we stick here to the original choice, as described in Table 2. The conjugating relation for the symmetry matrices may now be rewritten with the star operator as follows:

$$\begin{aligned} \overline{D_{\gamma\gamma'}^\Gamma}(R) &= D_{\gamma\gamma'}^\Gamma(R_0^{-1}RR_0) \\ &= \langle\Gamma\gamma|R_0^{-1}RR_0|\Gamma\gamma'\rangle \\ &= \langle\Gamma\gamma^*|R|\Gamma\gamma'^*\rangle \\ &= D_{\gamma^*\gamma'^*}^\Gamma(R) \end{aligned} \tag{13}$$

4 Coupling coefficients

The Clebsch-Gordan coupling coefficients of the type $\langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle$ describe how Γ_i and Γ_j representations combine to yield a resultant Γ .

$$|\Gamma \gamma\rangle = \sum_{\gamma_i \gamma_j} |\Gamma_i \gamma_i\rangle |\Gamma_j \gamma_j\rangle \langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle, \quad (14)$$

or vice-versa:

$$|\Gamma_i \gamma_i\rangle |\Gamma_j \gamma_j\rangle = \sum_{\Gamma \gamma} |\Gamma \gamma\rangle \langle \Gamma \gamma | \Gamma_i \gamma_i \Gamma_j \gamma_j \rangle \quad (15)$$

where the latter summation is over the direct product space $\Gamma_i \times \Gamma_j$. The coupling coefficients for the coupling between spin and orbital representations, using the complex components, have been published in earlier work [2]. Since all irreps involved were adapted to the fixed inner automorphism, described in (3), all coefficients can be chosen in *real* form [7]. Moreover they are invariant under permutation of Γ_i and Γ_j , for $\Gamma_i \neq \Gamma_j$. The coefficients appearing in the forward and backward coupling can thus be taken to be the same, or:

$$\langle \Gamma \gamma | \Gamma_i \gamma_i \Gamma_j \gamma_j \rangle = \langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle \quad (16)$$

The matrix elements of the linear Jahn-Teller Hamiltonian are as follows:

$$\mathcal{H}_{kl}(Q_{\Gamma_i \gamma_i}) = \sum_a \langle k | \frac{\partial \mathcal{H}}{\partial Q_{\Gamma_i \gamma_i}} | l \rangle_a Q_{\Gamma_i \gamma_i} \quad (17)$$

where the matrix element \mathcal{H}_{kl} is taken in the icosahedral origin, a is a multiplicity label which assigns two different direct product forms in the case of the h -modes. Since at present the coordinates are complex variables, one should take into account that the derivative with respect to the coordinate *transforms as the complex conjugate* of the coordinate.

$$\left| \frac{\partial \mathcal{H}}{\partial Q_{\Gamma_i \gamma_i}} \right| = |\overline{\Gamma_i \gamma_i}| \quad (18)$$

Following the Wigner-Eckart theorem, the matrix elements can now be factorised into a reduced matrix element, which is called the force element, and an appropriate coupling coefficient:

$$\langle k | \frac{\partial \mathcal{H}}{\partial Q_{\Gamma_i \gamma_i}} | l \rangle_a = F_{\Gamma_i}^a \langle \Gamma_9 k | \overline{\Gamma_i \gamma_i} | \Gamma_9 l \rangle_a \quad (19)$$

The complex conjugation can further be expressed with the help of the star operator. As indicated before, this will introduce a sign change for the G -type operators, and the JT matrix elements become:

$$\begin{aligned} \mathcal{H}_{kl}(\mathbf{Q}) = & -F_G \sum_{\gamma \in G} \langle \Gamma_9 k | G \gamma^* | \Gamma_9 l \rangle Q_{G \gamma} \\ & + F_{H_1} \sum_{\eta \in H} \langle \Gamma_9 k | H \eta^* | \Gamma_9 l \rangle_1 Q_{H \eta} + F_{H_2} \sum_{\eta \in H} \langle \Gamma_9 k | H \eta^* | \Gamma_9 l \rangle_2 Q_{H \eta} \end{aligned} \quad (20)$$

As it is written here, only one mode of h -symmetry is considered, but with two independent JT force elements, F_{H_1} and F_{H_2} , so that the multiplicity freedom of the coupling is covered. In a more general construction, one could introduce two different h -modes, one associated with the F_{H_1} coupling path, and

one described by F_{H_2} . It is unlikely that such modes which resolve the Jahn-Teller forces, will also be normal modes in the Hessian sense. Additional coupling terms thus will appear in the harmonic part of the Hamiltonian, which is however outside the scope of the present paper.

The previously obtained spin-orbit tables (most of which were only available as supplementary material) [2] contain the following products:

$$\begin{aligned} G \times \Gamma_9 &= 2\Gamma_9 \\ H \times \Gamma_9 &= 3\Gamma_9 \end{aligned} \quad (21)$$

which cover all possible couplings. In order to obtain the Jahn-Teller ones we have to convert these coupling tables into spin-spin couplings and verify which ones are antisymmetrised products. The switch from spin-orbit to spin-spin coupling coefficients can be performed by the following general formula [2]:

$$\dim(\Gamma)^{-\frac{1}{2}} \langle \Gamma_i \gamma_i \Gamma_j \gamma_j | \Gamma \gamma \rangle = \dim(\Gamma_j)^{-\frac{1}{2}} \langle \Gamma_i \gamma_i \Gamma \gamma^* | \Gamma_j \gamma_j^* \rangle \quad (22)$$

The starred components to the right can of course be expressed in unstarred ones, using the explicit forms of the inner automorphism. Applying this conversion to the two $G \times \Gamma_9$ spin-orbit tables, which are reproduced here as Tables 3 and 4, we verify that the multiplicity was separated on the basis of the product symmetrisation of the corresponding $\Gamma_9 \times \Gamma_9 = 2G$ spin-spin coupling. The coefficients in Table 3 refer to the antisymmetrised product, whereas Table 4 displays the symmetrised product. As an example with the help of Table 3 one may calculate the following permutations of spin-spin coupling coefficients:

$$\langle (-\frac{5}{2}) (\frac{5}{2}) | (i) \rangle = \frac{2}{\sqrt{6}} \langle (-\frac{5}{2}) (i)^* | (\frac{5}{2})^* \rangle = \frac{2}{\sqrt{6}} \langle (-\frac{5}{2}) (i) | (-\frac{5}{2}) \rangle = \frac{1}{4\sqrt{3}} \quad (23)$$

$$\langle (\frac{5}{2}) (-\frac{5}{2}) | (i) \rangle = \frac{2}{\sqrt{6}} \langle (\frac{5}{2}) (i)^* | (-\frac{5}{2})^* \rangle = -\frac{2}{\sqrt{6}} \langle (\frac{5}{2}) (i) | (\frac{5}{2}) \rangle = -\frac{1}{4\sqrt{3}} \quad (24)$$

which clearly shows the antisymmetrised nature of the product permutation.

In contrast the coupling in Table 4 corresponds to a symmetrised product, and thus is not JT-active.

$$\langle (\frac{5}{2}) (-\frac{1}{2}) | (i) \rangle = \frac{2}{\sqrt{6}} \langle (\frac{5}{2}) (i)^* | (-\frac{1}{2})^* \rangle = -\frac{2}{\sqrt{6}} \langle (\frac{5}{2}) (i) | (\frac{1}{2}) \rangle = -\frac{\sqrt{5}}{2\sqrt{6}} \quad (25)$$

$$\langle (-\frac{1}{2}) (\frac{5}{2}) | (i) \rangle = \frac{2}{\sqrt{6}} \langle (-\frac{1}{2}) (i)^* | (\frac{5}{2})^* \rangle = \frac{2}{\sqrt{6}} \langle (-\frac{1}{2}) (i) | (-\frac{5}{2}) \rangle = -\frac{\sqrt{5}}{2\sqrt{6}} \quad (26)$$

For the $H \times \Gamma_9$ coupling the published product separation was based on vector addition rules, which allow to differentiate between the three products by their spherical parentage:

$$H \times \Gamma_9 = \Gamma_9(5/2) + \Gamma_9(7/2) + \Gamma_9(9/2) \quad (27)$$

The $\Gamma_9(5/2)$ is antisymmetrised with respect to the permutation of the spin components and therefore suited for the JT-activity. We will associate with this coupling the F_{H1} reduced matrix element. It is listed in Table 5. On the other hand the remaining products $\Gamma_9(7/2)$ and $\Gamma_9(9/2)$ are found to be linear combinations of antisymmetric and symmetric couplings. The antisymmetric one can be deconvoluted by taking the following linear combination:

$$\Gamma_9(\text{antisym}) = \frac{\sqrt{2}}{3} \Gamma_9(7/2) - \frac{\sqrt{7}}{3} \Gamma_9(9/2) \quad (28)$$

Table 3. $G \otimes \Gamma_9 = \Gamma_9$ (antisymmetric product)

G	Γ_9	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
i	$\frac{5}{2}$	$\frac{1}{4\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot
i	$\frac{3}{2}$	\cdot	$\frac{-3}{4\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$
i	$\frac{1}{2}$	\cdot	\cdot	$\frac{1}{2\sqrt{2}}$	\cdot	\cdot	\cdot
i	$-\frac{1}{2}$	\cdot	\cdot	\cdot	$\frac{1}{2\sqrt{2}}$	\cdot	\cdot
i	$-\frac{3}{2}$	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{-3}{4\sqrt{2}}$	\cdot
i	$-\frac{5}{2}$	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{1}{4\sqrt{2}}$
0	$\frac{5}{2}$	\cdot	\cdot	$\frac{3}{8}$	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot
0	$\frac{3}{2}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{5}}{8}$	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$
0	$\frac{1}{2}$	$\frac{-3}{8}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{5}}{8}$	\cdot
0	$-\frac{1}{2}$	\cdot	$\frac{\sqrt{5}}{8}$	\cdot	\cdot	\cdot	$\frac{3}{8}$
0	$-\frac{3}{2}$	$\frac{-\sqrt{5}}{4\sqrt{2}}$	\cdot	$\frac{\sqrt{5}}{8}$	\cdot	\cdot	\cdot
0	$-\frac{5}{2}$	\cdot	$\frac{-\sqrt{5}}{4\sqrt{2}}$	\cdot	$\frac{-3}{8}$	\cdot	\cdot
1	$\frac{5}{2}$	\cdot	$\frac{1}{8}$	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	\cdot
1	$\frac{3}{2}$	$\frac{-\sqrt{5}}{8}$	\cdot	$\frac{-\sqrt{5}}{8\sqrt{2}}$	\cdot	\cdot	\cdot
1	$\frac{1}{2}$	\cdot	$\frac{5}{8\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{5}}{8\sqrt{2}}$
1	$-\frac{1}{2}$	$\frac{7}{8\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot
1	$-\frac{3}{2}$	\cdot	\cdot	\cdot	$\frac{-5}{8\sqrt{2}}$	\cdot	$\frac{-1}{8}$
1	$-\frac{5}{2}$	\cdot	\cdot	$\frac{-7}{8\sqrt{2}}$	\cdot	$\frac{\sqrt{5}}{8}$	\cdot
-1	$\frac{5}{2}$	\cdot	$\frac{-\sqrt{5}}{8}$	\cdot	$\frac{7}{8\sqrt{2}}$	\cdot	\cdot
-1	$\frac{3}{2}$	$\frac{1}{8}$	\cdot	$\frac{5}{8\sqrt{2}}$	\cdot	\cdot	\cdot
-1	$\frac{1}{2}$	\cdot	$\frac{-\sqrt{5}}{8\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{-7}{8\sqrt{2}}$
-1	$-\frac{1}{2}$	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{-5}{8\sqrt{2}}$	\cdot
-1	$-\frac{3}{2}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{\sqrt{5}}{8}$
-1	$-\frac{5}{2}$	\cdot	\cdot	$\frac{-\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{-1}{8}$	\cdot

This product is shown in Table 6. We will associate with this coupling the F_{H2} reduced matrix element. For completeness, we also provide the complementary symmetric product, which is non JT-active, in Table 7.

$$\Gamma_9(sym) = \frac{\sqrt{7}}{3}\Gamma_9(7/2) + \frac{\sqrt{2}}{3}\Gamma_9(9/2) \tag{29}$$

5 Construction of the Hamiltonian

We are now in a position to construct the full JT Hamiltonian, by inserting the coupling coefficients of Tables 3, 5 and 6 in (20), taking into account the star operator forms as described in (10). As an example let us construct the first entry of the G -matrix.

$$\mathcal{H}_{11}(\mathbf{Q}_G) = -F_G \langle (\frac{5}{2}) | (i)^* (\frac{5}{2}) \rangle Q_{Gi} = -\frac{i}{4\sqrt{2}} F_G Q_{Ga} \tag{30}$$

Table 4. $G \otimes \Gamma_9 = \Gamma_9$ (symmetric product)

G	Γ_9	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
i	$\frac{5}{2}$	\cdot	\cdot	$\frac{\sqrt{5}}{4}$	\cdot	\cdot	\cdot
i	$\frac{3}{2}$	\cdot	\cdot	\cdot	$\frac{1}{4}$	\cdot	\cdot
i	$\frac{1}{2}$	$\frac{\sqrt{5}}{4}$	\cdot	\cdot	\cdot	$\frac{-1}{4}$	\cdot
i	$-\frac{1}{2}$	\cdot	$\frac{-1}{4}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{5}}{4}$
i	$-\frac{3}{2}$	\cdot	\cdot	$\frac{1}{4}$	\cdot	\cdot	\cdot
i	$-\frac{5}{2}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{4}$	\cdot	\cdot
0	$\frac{5}{2}$	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{8}$	\cdot	\cdot	\cdot
0	$\frac{3}{2}$	\cdot	$\frac{-7}{4\sqrt{10}}$	\cdot	$\frac{-1}{8}$	\cdot	\cdot
0	$\frac{1}{2}$	$\frac{-\sqrt{5}}{8}$	\cdot	$\frac{-1}{\sqrt{10}}$	\cdot	$\frac{1}{8}$	\cdot
0	$-\frac{1}{2}$	\cdot	$\frac{-1}{8}$	\cdot	$\frac{1}{\sqrt{10}}$	\cdot	$\frac{\sqrt{5}}{8}$
0	$-\frac{3}{2}$	\cdot	\cdot	$\frac{1}{8}$	\cdot	$\frac{7}{4\sqrt{10}}$	\cdot
0	$-\frac{5}{2}$	\cdot	\cdot	\cdot	$\frac{\sqrt{5}}{8}$	\cdot	$\frac{-\sqrt{5}}{4\sqrt{2}}$
1	$\frac{5}{2}$	\cdot	$\frac{-\sqrt{5}}{8}$	\cdot	$\frac{-5}{8\sqrt{2}}$	\cdot	\cdot
1	$\frac{3}{2}$	$\frac{3}{8}$	\cdot	$\frac{1}{8\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{4}$	\cdot
1	$\frac{1}{2}$	\cdot	$\frac{-3}{8\sqrt{10}}$	\cdot	$\frac{1}{4}$	\cdot	$\frac{-5}{8\sqrt{2}}$
1	$-\frac{1}{2}$	$\frac{-\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{-3}{4\sqrt{5}}$	\cdot	$\frac{1}{8\sqrt{2}}$	\cdot
1	$-\frac{3}{2}$	\cdot	$\frac{-1}{4}$	\cdot	$\frac{-3}{8\sqrt{10}}$	\cdot	$\frac{-\sqrt{5}}{8}$
1	$-\frac{5}{2}$	\cdot	\cdot	$\frac{-\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{3}{8}$	\cdot
-1	$\frac{5}{2}$	\cdot	$\frac{-3}{8}$	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	\cdot
-1	$\frac{3}{2}$	$\frac{\sqrt{5}}{8}$	\cdot	$\frac{3}{8\sqrt{10}}$	\cdot	$\frac{1}{4}$	\cdot
-1	$\frac{1}{2}$	\cdot	$\frac{-1}{8\sqrt{2}}$	\cdot	$\frac{3}{4\sqrt{5}}$	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$
-1	$-\frac{1}{2}$	$\frac{5}{8\sqrt{2}}$	\cdot	$\frac{-1}{4}$	\cdot	$\frac{3}{8\sqrt{10}}$	\cdot
-1	$-\frac{3}{2}$	\cdot	$\frac{\sqrt{5}}{4}$	\cdot	$\frac{-1}{8\sqrt{2}}$	\cdot	$\frac{-3}{8}$
-1	$-\frac{5}{2}$	\cdot	\cdot	$\frac{5}{8\sqrt{2}}$	\cdot	$\frac{\sqrt{5}}{8}$	\cdot

where we have converted the coordinate back into real form. Since the Hamiltonian is hermitian a diagonal matrix element is expected to be real. In fact the coupling coefficients are defined up to an overall external phase factor, and we can always take out this imaginary phase, e.g. by multiplying the entire G -matrix by the imaginary i . Formally this means that a factor $-i$ is absorbed into the reduced matrix element, say $\tilde{F}_G = -iF_G$. The previous equation then becomes:

$$\mathcal{H}_{11}(\mathbf{Q}_G) = \frac{1}{4\sqrt{2}} \tilde{F}_G Q_{Ga} \quad (31)$$

To check the hermiticity let us further calculate the 12 and 21 elements:

$$\begin{aligned} \mathcal{H}_{12}(\mathbf{Q}_G) &= -F_G \langle (\frac{5}{2}) | (1)^* (\frac{3}{2}) \rangle Q_{G1} - F_G \langle (\frac{5}{2}) | (-1)^* (\frac{3}{2}) \rangle Q_{G-1} \\ &= \tilde{F}_G \left[\frac{i\phi}{4\sqrt{2}} Q_{Gx} + \frac{\phi^{-1}}{4\sqrt{2}} Q_{Gy} \right] \\ \mathcal{H}_{21}(\mathbf{Q}_G) &= -F_G \langle (\frac{3}{2}) | (1)^* (\frac{5}{2}) \rangle Q_{G1} - F_G \langle (\frac{3}{2}) | (-1)^* (\frac{5}{2}) \rangle Q_{G-1} \\ &= \tilde{F}_G \left[\frac{-i\phi}{4\sqrt{2}} Q_{Gx} + \frac{\phi^{-1}}{4\sqrt{2}} Q_{Gy} \right] \end{aligned} \quad (32)$$

Table 5. $H \otimes \Gamma_9 = \Gamma_9 (J = \frac{5}{2})$ (antisymmetric product)

H	Γ_9	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
2	$\frac{5}{2}$
2	$\frac{3}{2}$
2	$\frac{1}{2}$	$\frac{-\sqrt{3}}{\sqrt{14}}$
2	$-\frac{1}{2}$.	$\frac{-3\sqrt{3}}{\sqrt{70}}$
2	$-\frac{3}{2}$.	.	$\frac{-3\sqrt{3}}{\sqrt{70}}$.	.	.
2	$-\frac{5}{2}$.	.	.	$\frac{-\sqrt{3}}{\sqrt{14}}$.	.
-2	$\frac{5}{2}$.	.	$\frac{-\sqrt{3}}{\sqrt{14}}$.	.	.
-2	$\frac{3}{2}$.	.	.	$\frac{-3\sqrt{3}}{\sqrt{70}}$.	.
-2	$\frac{1}{2}$	$\frac{-3\sqrt{3}}{\sqrt{70}}$.
-2	$-\frac{1}{2}$	$\frac{-\sqrt{3}}{\sqrt{14}}$
-2	$-\frac{3}{2}$
-2	$-\frac{5}{2}$
1	$\frac{5}{2}$
1	$\frac{3}{2}$	$\frac{\sqrt{3}}{\sqrt{7}}$
1	$\frac{1}{2}$.	$\frac{\sqrt{6}}{\sqrt{35}}$
1	$-\frac{1}{2}$
1	$-\frac{3}{2}$.	.	.	$\frac{-\sqrt{6}}{\sqrt{35}}$.	.
1	$-\frac{5}{2}$	$\frac{-\sqrt{3}}{\sqrt{7}}$.
-1	$\frac{5}{2}$.	$\frac{-\sqrt{3}}{\sqrt{7}}$
-1	$\frac{3}{2}$.	.	$\frac{-\sqrt{6}}{\sqrt{35}}$.	.	.
-1	$\frac{1}{2}$
-1	$-\frac{1}{2}$	$\frac{\sqrt{6}}{\sqrt{35}}$.
-1	$-\frac{3}{2}$	$\frac{\sqrt{3}}{\sqrt{7}}$
-1	$-\frac{5}{2}$
0	$\frac{5}{2}$	$\frac{-\sqrt{5}}{\sqrt{14}}$
0	$\frac{3}{2}$.	$\frac{1}{\sqrt{70}}$
0	$\frac{1}{2}$.	.	$\frac{2\sqrt{2}}{\sqrt{35}}$.	.	.
0	$-\frac{1}{2}$.	.	.	$\frac{2\sqrt{2}}{\sqrt{35}}$.	.
0	$-\frac{3}{2}$	$\frac{1}{\sqrt{70}}$.
0	$-\frac{5}{2}$	$\frac{-\sqrt{5}}{\sqrt{14}}$

which is nicely hermitian; ϕ is the golden number. In the sequel we will drop the tilde on F_G .

The matrix elements for the H -part can be calculated in the same way. In this case the resulting matrices appear to be hermitian without further tilde operation. A few elements are calculated here for illustration:

$$\mathcal{H}_{23}^1(\mathbf{Q}_H) = F_{H_1} \langle (\frac{3}{2}) | (-1)^* (\frac{1}{2}) \rangle_1 Q_{H-1} = -\frac{\sqrt{3}}{\sqrt{35}} F_{H_1} [-iQ_{Hx} + Q_{Hy}]$$

$$\mathcal{H}_{35}^1(\mathbf{Q}_H) = F_{H_1} \langle (\frac{1}{2}) | (-2)^* (-\frac{3}{2}) \rangle_1 Q_{H-2}$$

$$= -\frac{3\sqrt{3}}{4\sqrt{70}} F_{H_1} (\sqrt{5}Q_{H\theta} + \sqrt{3}Q_{H\epsilon} - i\sqrt{8}Q_{Hz})$$

$$\begin{aligned}
 \mathcal{H}_{44}^2(Q_H) &= F_{H_2} \langle (-\frac{1}{2}) | (-2)^* (-\frac{1}{2}) \rangle_2 Q_{H-2} + F_{H_2} \langle (-\frac{1}{2}) | (2)^* (-\frac{1}{2}) \rangle_2 Q_{H2} \\
 &\quad + F_{H_2} \langle (-\frac{1}{2}) | (0)^* (-\frac{1}{2}) \rangle_2 Q_{H0} \\
 &= \frac{\sqrt{5}}{8\sqrt{7}} Q_{H\theta} + \frac{3\sqrt{3}}{8\sqrt{7}} Q_{H\epsilon}
 \end{aligned}
 \tag{33}$$

Table 6. $H \otimes \Gamma_9 = \Gamma_9[\frac{\sqrt{2}}{3}(J = \frac{7}{2}) - \frac{\sqrt{7}}{3}(J = \frac{9}{2})]$ (antisymmetric)

H	Γ_9	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
2	$\frac{5}{2}$	$\frac{\sqrt{7}}{32}$.	$\frac{3\sqrt{7}}{16\sqrt{2}}$.	$\frac{-3\sqrt{35}}{32}$.
2	$\frac{3}{2}$.	$\frac{-3\sqrt{7}}{32}$.	$\frac{-\sqrt{35}}{16\sqrt{2}}$.	$\frac{-3\sqrt{35}}{32}$
2	$\frac{1}{2}$	$\frac{-3}{16\sqrt{14}}$.	$\frac{\sqrt{7}}{16}$.	$\frac{-\sqrt{35}}{16\sqrt{2}}$.
2	$-\frac{1}{2}$.	$\frac{\sqrt{5}}{16\sqrt{14}}$.	$\frac{\sqrt{7}}{16}$.	$\frac{3\sqrt{7}}{16\sqrt{2}}$
2	$-\frac{3}{2}$	$\frac{\sqrt{7}}{32\sqrt{5}}$.	$\frac{\sqrt{5}}{16\sqrt{14}}$.	$\frac{-3\sqrt{7}}{32}$.
2	$-\frac{5}{2}$.	$\frac{\sqrt{7}}{32\sqrt{5}}$.	$\frac{-3}{16\sqrt{14}}$.	$\frac{\sqrt{7}}{32}$
-2	$\frac{5}{2}$	$\frac{\sqrt{7}}{32}$.	$\frac{-3}{16\sqrt{14}}$.	$\frac{\sqrt{7}}{32\sqrt{5}}$.
-2	$\frac{3}{2}$.	$\frac{-3\sqrt{7}}{32}$.	$\frac{\sqrt{5}}{16\sqrt{14}}$.	$\frac{\sqrt{7}}{32\sqrt{5}}$
-2	$\frac{1}{2}$	$\frac{3\sqrt{7}}{16\sqrt{2}}$.	$\frac{\sqrt{7}}{16}$.	$\frac{\sqrt{5}}{16\sqrt{14}}$.
-2	$-\frac{1}{2}$.	$\frac{-\sqrt{35}}{16\sqrt{2}}$.	$\frac{\sqrt{7}}{16}$.	$\frac{-3}{16\sqrt{14}}$
-2	$-\frac{3}{2}$	$\frac{-3\sqrt{35}}{32}$.	$\frac{-\sqrt{35}}{16\sqrt{2}}$.	$\frac{-3\sqrt{7}}{32}$.
-2	$-\frac{5}{2}$.	$\frac{-3\sqrt{35}}{32}$.	$\frac{3\sqrt{7}}{16\sqrt{2}}$.	$\frac{\sqrt{7}}{32}$
1	$\frac{5}{2}$.	$\frac{-\sqrt{7}}{4\sqrt{5}}$.	$\frac{-\sqrt{7}}{4\sqrt{2}}$.	.
1	$\frac{3}{2}$	$\frac{-1}{4\sqrt{7}}$.	$\frac{\sqrt{7}}{4\sqrt{2}}$.	.	.
1	$\frac{1}{2}$.	$\frac{\sqrt{5}}{4\sqrt{14}}$.	.	.	$\frac{\sqrt{7}}{4\sqrt{2}}$
1	$-\frac{1}{2}$	$\frac{\sqrt{7}}{4\sqrt{10}}$.	.	.	$\frac{-\sqrt{7}}{4\sqrt{2}}$.
1	$-\frac{3}{2}$.	.	.	$\frac{-\sqrt{5}}{4\sqrt{14}}$.	$\frac{\sqrt{7}}{4\sqrt{5}}$
1	$-\frac{5}{2}$.	.	$\frac{-\sqrt{7}}{4\sqrt{10}}$.	$\frac{1}{4\sqrt{7}}$.
-1	$\frac{5}{2}$.	$\frac{1}{4\sqrt{7}}$.	$\frac{-\sqrt{7}}{4\sqrt{10}}$.	.
-1	$\frac{3}{2}$	$\frac{\sqrt{7}}{4\sqrt{5}}$.	$\frac{-\sqrt{5}}{4\sqrt{14}}$.	.	.
-1	$\frac{1}{2}$.	$\frac{-\sqrt{7}}{4\sqrt{2}}$.	.	.	$\frac{\sqrt{7}}{4\sqrt{10}}$
-1	$-\frac{1}{2}$	$\frac{\sqrt{7}}{4\sqrt{2}}$.	.	.	$\frac{\sqrt{5}}{4\sqrt{14}}$.
-1	$-\frac{3}{2}$.	.	.	$\frac{\sqrt{7}}{4\sqrt{2}}$.	$\frac{-1}{4\sqrt{7}}$
-1	$-\frac{5}{2}$.	.	$\frac{-\sqrt{7}}{4\sqrt{2}}$.	$\frac{-\sqrt{7}}{4\sqrt{5}}$.
0	$\frac{5}{2}$	$\frac{-\sqrt{15}}{16\sqrt{14}}$.	$\frac{3\sqrt{21}}{16\sqrt{5}}$.	$\frac{\sqrt{21}}{16\sqrt{2}}$.
0	$\frac{3}{2}$.	$\frac{3\sqrt{15}}{16\sqrt{14}}$.	$\frac{-\sqrt{21}}{16}$.	$\frac{\sqrt{21}}{16\sqrt{2}}$
0	$\frac{1}{2}$	$\frac{3\sqrt{21}}{16\sqrt{5}}$.	$\frac{-\sqrt{15}}{8\sqrt{14}}$.	$\frac{-\sqrt{21}}{16}$.
0	$-\frac{1}{2}$.	$\frac{-\sqrt{21}}{16}$.	$\frac{-\sqrt{15}}{8\sqrt{14}}$.	$\frac{3\sqrt{21}}{16\sqrt{5}}$
0	$-\frac{3}{2}$	$\frac{\sqrt{21}}{16\sqrt{2}}$.	$\frac{-\sqrt{21}}{16}$.	$\frac{3\sqrt{15}}{16\sqrt{14}}$.
0	$-\frac{5}{2}$.	$\frac{\sqrt{21}}{16\sqrt{2}}$.	$\frac{3\sqrt{21}}{16\sqrt{5}}$.	$\frac{-\sqrt{15}}{16\sqrt{14}}$

Table 7. $H \otimes \Gamma_9 = \Gamma_9[\frac{\sqrt{7}}{3}(J = \frac{7}{2}) + \frac{\sqrt{2}}{3}(J = \frac{9}{2})]$ (symmetric)

H		Γ_9					
Γ_9		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
2	$\frac{5}{2}$	$\frac{-1}{16\sqrt{2}}$	\cdot	$\frac{-3}{16}$	\cdot	$\frac{3\sqrt{5}}{16\sqrt{2}}$	\cdot
2	$\frac{3}{2}$	\cdot	$\frac{5}{16\sqrt{2}}$	\cdot	$\frac{3\sqrt{5}}{16}$	\cdot	$\frac{-3\sqrt{5}}{16\sqrt{2}}$
2	$\frac{1}{2}$	$\frac{1}{16}$	\cdot	$\frac{-5}{8\sqrt{2}}$	\cdot	$\frac{-3\sqrt{5}}{16}$	\cdot
2	$-\frac{1}{2}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot	$\frac{5}{8\sqrt{2}}$	\cdot	$\frac{3}{16}$
2	$-\frac{3}{2}$	$\frac{-9}{16\sqrt{10}}$	\cdot	$\frac{\sqrt{5}}{16}$	\cdot	$\frac{-5}{16\sqrt{2}}$	\cdot
2	$-\frac{5}{2}$	\cdot	$\frac{9}{16\sqrt{10}}$	\cdot	$\frac{-1}{16}$	\cdot	$\frac{1}{16\sqrt{2}}$
-2	$\frac{5}{2}$	$\frac{1}{16\sqrt{2}}$	\cdot	$\frac{-1}{16}$	\cdot	$\frac{9}{16\sqrt{10}}$	\cdot
-2	$\frac{3}{2}$	\cdot	$\frac{-5}{16\sqrt{2}}$	\cdot	$\frac{\sqrt{5}}{16}$	\cdot	$\frac{-9}{16\sqrt{10}}$
-2	$\frac{1}{2}$	$\frac{3}{16}$	\cdot	$\frac{5}{8\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot
-2	$-\frac{1}{2}$	\cdot	$\frac{-3\sqrt{5}}{16}$	\cdot	$\frac{-5}{8\sqrt{2}}$	\cdot	$\frac{1}{16}$
-2	$-\frac{3}{2}$	$\frac{-3\sqrt{5}}{16\sqrt{2}}$	\cdot	$\frac{3\sqrt{5}}{16}$	\cdot	$\frac{5}{16\sqrt{2}}$	\cdot
-2	$-\frac{5}{2}$	\cdot	$\frac{3\sqrt{5}}{16\sqrt{2}}$	\cdot	$\frac{-3}{16}$	\cdot	$\frac{-1}{16\sqrt{2}}$
1	$\frac{5}{2}$	\cdot	$\frac{3}{16\sqrt{10}}$	\cdot	$\frac{-1}{16}$	\cdot	$\frac{15}{16\sqrt{2}}$
1	$\frac{3}{2}$	$\frac{1}{16\sqrt{2}}$	\cdot	$\frac{-3}{16}$	\cdot	$\frac{\sqrt{5}}{16\sqrt{2}}$	\cdot
1	$\frac{1}{2}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot	$\frac{3}{8\sqrt{2}}$	\cdot	$\frac{-1}{16}$
1	$-\frac{1}{2}$	$\frac{-11}{16\sqrt{5}}$	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{-3}{16}$	\cdot
1	$-\frac{3}{2}$	\cdot	$\frac{11}{16\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot	$\frac{3}{16\sqrt{10}}$
1	$-\frac{5}{2}$	$\frac{-3\sqrt{5}}{16\sqrt{2}}$	\cdot	$\frac{-11}{16\sqrt{5}}$	\cdot	$\frac{1}{16\sqrt{2}}$	\cdot
-1	$\frac{5}{2}$	\cdot	$\frac{1}{16\sqrt{2}}$	\cdot	$\frac{-11}{16\sqrt{5}}$	\cdot	$\frac{-3\sqrt{5}}{16\sqrt{2}}$
-1	$\frac{3}{2}$	$\frac{3}{16\sqrt{10}}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot	$\frac{11}{16\sqrt{2}}$	\cdot
-1	$\frac{1}{2}$	\cdot	$\frac{-3}{16}$	\cdot	$\frac{\sqrt{5}}{8\sqrt{2}}$	\cdot	$\frac{-11}{16\sqrt{5}}$
-1	$-\frac{1}{2}$	$\frac{-1}{16}$	\cdot	$\frac{3}{8\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{16}$	\cdot
-1	$-\frac{3}{2}$	\cdot	$\frac{\sqrt{5}}{16\sqrt{2}}$	\cdot	$\frac{-3}{16}$	\cdot	$\frac{1}{16\sqrt{2}}$
-1	$-\frac{5}{2}$	$\frac{15}{16\sqrt{2}}$	\cdot	$\frac{-1}{16}$	\cdot	$\frac{3}{16\sqrt{10}}$	\cdot
0	$\frac{5}{2}$	\cdot	\cdot	$\frac{\sqrt{3}}{4\sqrt{10}}$	\cdot	$\frac{\sqrt{3}}{4}$	\cdot
0	$\frac{3}{2}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{3}}{4\sqrt{2}}$	\cdot	$\frac{-\sqrt{3}}{4}$
0	$\frac{1}{2}$	$\frac{-\sqrt{3}}{4\sqrt{10}}$	\cdot	\cdot	\cdot	$\frac{\sqrt{3}}{4\sqrt{2}}$	\cdot
0	$-\frac{1}{2}$	\cdot	$\frac{\sqrt{3}}{4\sqrt{2}}$	\cdot	\cdot	\cdot	$\frac{-\sqrt{3}}{4\sqrt{10}}$
0	$-\frac{3}{2}$	$\frac{-\sqrt{3}}{4}$	\cdot	$\frac{-\sqrt{3}}{4\sqrt{2}}$	\cdot	\cdot	\cdot
0	$-\frac{5}{2}$	\cdot	$\frac{\sqrt{3}}{4}$	\cdot	$\frac{\sqrt{3}}{4\sqrt{10}}$	\cdot	\cdot

The linear JT matrix is symplectic because of the time reversal symmetry [1]. This implies that it has the following general form:

$$\mathcal{H}_F = \begin{pmatrix} \frac{k}{\sqrt{3}} + l & \mu & \nu & \sigma & \tau & 0 \\ \mu^* & \frac{k}{\sqrt{3}} - l & \kappa & \lambda & 0 & \tau \\ \nu^* & \kappa^* & \frac{-2k}{\sqrt{3}} & 0 & \lambda & -\sigma \\ \sigma^* & \lambda^* & 0 & \frac{-2k}{\sqrt{3}} & -\kappa & \nu \\ \tau^* & 0 & \lambda^* & -\kappa^* & \frac{k}{\sqrt{3}} - l & -\mu \\ 0 & \tau^* & -\sigma^* & \nu^* & -\mu^* & \frac{k}{\sqrt{3}} + l \end{pmatrix} \quad (34)$$

This matrix contains eight parameters. The two parameters on the diagonal, k and l , are real while there are six off-diagonal parameters, indicated by Greek symbols, which are complex. This yields a total of 14 variables, matching the full freedom of the $g \oplus 2h$ distortion space, in the case where the h -couplings are assigned to two different h -modes. The 14 Hamiltonian parameters are related to the linear JT matrix elements as follows:

$$\begin{aligned} k &= -\frac{\sqrt{6}}{8} F_G Q_{Ga} + \frac{3}{2\sqrt{35}} F_{H_1} (-Q_{H\theta} + \frac{\sqrt{5}}{\sqrt{3}} Q_{H\epsilon}) \\ &\quad - \frac{\sqrt{15}}{16\sqrt{7}} F_{H_2} (Q_{H\theta} + \frac{3\sqrt{3}}{\sqrt{5}} Q_{H\epsilon}) \\ l &= \frac{1}{2\sqrt{2}} F_G Q_{Ga} + \frac{3\sqrt{3}}{4\sqrt{35}} F_{H_1} (-Q_{H\theta} + \frac{\sqrt{5}}{\sqrt{3}} Q_{H\epsilon}) \\ &\quad + \frac{\sqrt{5}}{8\sqrt{7}} F_{H_2} (Q_{H\theta} + \frac{3\sqrt{3}}{\sqrt{5}} Q_{H\epsilon}) \\ \Re(\mu) &= \frac{\phi^{-1}}{4\sqrt{2}} F_G Q_{Gy} - \frac{\sqrt{3}}{\sqrt{14}} F_{H_1} Q_{Hy} + \frac{\sqrt{5}\phi + 1}{2\sqrt{70}} F_{H_2} Q_{Hy} \\ \Im(\mu) &= \frac{\phi}{4\sqrt{2}} F_G Q_{Gx} + \frac{\sqrt{3}}{\sqrt{14}} F_{H_1} Q_{Hx} + \frac{\sqrt{5}\phi^{-1} + 1}{2\sqrt{70}} F_{H_2} Q_{Hx} \\ \Re(\nu) &= -\frac{\sqrt{15}}{4\sqrt{14}} F_{H_1} (Q_{H\theta} + \frac{\sqrt{3}}{\sqrt{5}} Q_{H\epsilon}) + \frac{27}{8\sqrt{70}} F_{H_2} (Q_{H\theta} - \frac{\sqrt{5}}{3\sqrt{3}} Q_{H\epsilon}) \\ \Im(\nu) &= -\frac{3}{8} F_G Q_{Gz} + \frac{\sqrt{3}}{2\sqrt{7}} F_{H_1} Q_{Hz} + \frac{3}{4\sqrt{7}} F_{H_2} Q_{Hz} \\ \Re(\sigma) &= -\frac{\sqrt{5}\phi + 1}{8} F_G Q_{Gy} + \frac{\sqrt{7}\phi^{-1}}{4\sqrt{5}} F_{H_2} Q_{Hy} \\ \Im(\sigma) &= -\frac{\sqrt{5}\phi^{-1} + 1}{8} F_G Q_{Gx} + \frac{\sqrt{7}\phi}{4\sqrt{5}} F_{H_2} Q_{Hx} \\ \Re(\tau) &= \frac{\sqrt{5}}{4\sqrt{2}} F_G Q_{Ga} - \frac{\sqrt{7}}{16} F_{H_2} (Q_{H\theta} + \frac{3\sqrt{3}}{\sqrt{5}} Q_{H\epsilon}) \\ \Im(\tau) &= -\frac{\sqrt{5}}{4\sqrt{2}} F_G Q_{Gz} - \frac{\sqrt{7}}{2\sqrt{10}} F_{H_2} Q_{Hz} \\ \Re(\kappa) &= -\frac{\sqrt{5}\phi^{-1}}{8} F_G Q_{Gy} - \frac{\sqrt{3}}{\sqrt{35}} F_{H_1} Q_{Hy} - \frac{\sqrt{5}\phi + 1}{4\sqrt{7}} F_{H_2} Q_{Hy} \end{aligned}$$

$$\begin{aligned}
\Im(\kappa) &= -\frac{\sqrt{5}\phi}{8}F_GQ_{Gx} + \frac{\sqrt{3}}{\sqrt{35}}F_{H_1}Q_{Hx} - \frac{\sqrt{5}\phi^{-1} + 1}{4\sqrt{7}}F_{H_2}Q_{Hx} \\
\Re(\lambda) &= -\frac{3\sqrt{3}}{4\sqrt{14}}F_{H_1}(Q_{H\theta} + \frac{\sqrt{3}}{\sqrt{5}}Q_{H\epsilon}) + \frac{9}{8\sqrt{14}}F_{H_2}(-Q_{H\theta} + \frac{\sqrt{5}}{3\sqrt{3}}Q_{H\epsilon}) \\
\Im(\lambda) &= \frac{\sqrt{5}}{8}F_GQ_{Gz} + \frac{3\sqrt{3}}{2\sqrt{35}}F_{H_1}Q_{Hz} - \frac{\sqrt{5}}{4\sqrt{7}}F_{H_2}Q_{Hz}
\end{aligned} \tag{35}$$

The resulting matrix has icosahedral symmetry. This forms an important validity check of the coupling coefficients. The study of its roots and principal distortion schemes is dealt with in a separate paper [1].

6 Special coupling cases

Group theory reveals that there are two cases where the manifold of the icosahedral sextet coincides with the coupling space of an orbital triplet with a spin doublet. These two cases are:

$$\begin{aligned}
\Gamma_9 &= T_1 \times \Gamma_7 \\
\Gamma_9 &= T_2 \times \Gamma_6
\end{aligned} \tag{36}$$

where Γ_6 and Γ_7 are twofold degenerate spin representations, also sometimes referred to as E' and E'' resp. Sextet components which are constructed in this way, will contain a spin and an orbital part, and their JT activity may be attributed to the instability of the underlying orbital triplet, of the $T \times h$ type [8], [9]. This gives rise to special $\Gamma_9 \times h$ Hamiltonians. The Γ_9 components can be written as a sum over coupled terms, according to the coupling tables for the respective products (see Tables 8 and 9). JT matrix elements between these coupled states are entirely attributed to the constituent orbital parts, multiplied by a spin overlap factor $\langle \sigma' | \sigma \rangle = \delta_{\sigma' \sigma}$. The basic Hamiltonian matrices for the orbital triplet terms are given below. In the case of a T_1 term, with components ordered as $|T_1x\rangle, |T_1y\rangle, |T_1z\rangle$, the linear Hamiltonian reads:

$$k_{T_1} \begin{pmatrix} \frac{\sqrt{3}}{2\phi\sqrt{5}}Q_{H\theta} + \frac{\phi^2}{2\sqrt{5}}Q_{H\epsilon} & \frac{\sqrt{3}}{\sqrt{10}}Q_{Hz} & \frac{\sqrt{3}}{\sqrt{10}}Q_{Hy} \\ \frac{\sqrt{3}}{\sqrt{10}}Q_{Hz} & \frac{-\phi\sqrt{3}}{2\sqrt{5}}Q_{H\theta} + \frac{-1}{2\phi^2\sqrt{5}}Q_{H\epsilon} & \frac{\sqrt{3}}{\sqrt{10}}Q_{Hx} \\ \frac{\sqrt{3}}{\sqrt{10}}Q_{Hy} & \frac{\sqrt{3}}{\sqrt{10}}Q_{Hx} & \frac{\sqrt{3}}{2\sqrt{5}}Q_{H\theta} - \frac{1}{2}Q_{H\epsilon} \end{pmatrix} \tag{37}$$

Table 8. $T_1 \otimes \Gamma_7 = \Gamma_9$

T_1	Γ_7	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
0	α	$\frac{3}{4\sqrt{2}}$	\cdot	$-\frac{3}{4}$	\cdot	$-\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot
0	β	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	$\frac{3}{4}$	\cdot	$-\frac{3}{4\sqrt{2}}$
1	α	\cdot	$\frac{3}{8}$	\cdot	$\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	$\frac{3\sqrt{5}}{8}$
1	β	$-\frac{1}{8}$	\cdot	$-\frac{3}{4\sqrt{2}}$	\cdot	$\frac{3\sqrt{5}}{8}$	\cdot
-1	α	\cdot	$-\frac{3\sqrt{5}}{8}$	\cdot	$\frac{3}{4\sqrt{2}}$	\cdot	$\frac{1}{8}$
-1	β	$-\frac{3\sqrt{5}}{8}$	\cdot	$-\frac{\sqrt{5}}{4\sqrt{2}}$	\cdot	$-\frac{3}{8}$	\cdot

Similarly, for the T_2 , ordered likewise, one has:

$$k_{T_2} \begin{pmatrix} \frac{\phi\sqrt{3}}{2\sqrt{5}}Q_{H\theta} - \frac{1}{2\phi^2\sqrt{5}}Q_{H\epsilon} & -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hz} & -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hy} \\ -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hz} & \frac{-\sqrt{3}}{2\phi\sqrt{5}}Q_{H\theta} + \frac{\phi^2}{2\sqrt{5}}Q_{H\epsilon} & -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hx} \\ -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hy} & -\frac{\sqrt{3}}{\sqrt{10}}Q_{Hx} & -\frac{\sqrt{3}}{2\sqrt{5}}Q_{H\theta} - \frac{1}{2}Q_{H\epsilon} \end{pmatrix} \quad (38)$$

As an example, let us calculate the \mathcal{H}_{11} matrix element for a sextet term which is obtained by coupling $T_1 \times \Gamma_7$. From Table 8 the $|5/2\rangle$ component is given by:

$$\begin{aligned} |5/2\rangle &= \frac{3}{4\sqrt{2}}|0\rangle|\alpha\rangle - \frac{1}{8}|1\rangle|\beta\rangle - \frac{3\sqrt{5}}{8}|-1\rangle|\beta\rangle \\ &= \frac{3}{4\sqrt{2}}|z\rangle|\alpha\rangle + \frac{1-3\sqrt{5}}{8\sqrt{2}}|x\rangle|\beta\rangle + i\frac{1+3\sqrt{5}}{8\sqrt{2}}|y\rangle|\beta\rangle \end{aligned} \quad (39)$$

where we have returned to the real basis with the help of Table 2. Combining this result now with the JT matrix elements for $T_1 \times h$ in (37), keeping in mind that the $|\alpha\rangle$ and $|\beta\rangle$ pseudo-spins are orthogonal to each other, one obtains:

$$\begin{aligned} \mathcal{H}_{11} &= \frac{9}{32}\langle z|\mathcal{H}|z\rangle + \frac{23-3\sqrt{5}}{64}\langle x|\mathcal{H}|x\rangle + \frac{23+3\sqrt{5}}{64}\langle y|\mathcal{H}|y\rangle \\ &\quad + i\frac{11}{32}[\langle y|\mathcal{H}|x\rangle - \langle x|\mathcal{H}|y\rangle] \\ &= k_{T_1} \left(-\frac{\sqrt{15}}{32}Q_{H\theta} - \frac{1}{32}Q_{H\epsilon} \right) \end{aligned} \quad (40)$$

This expression should be compared with the corresponding matrix element for the general Hamiltonian in h -space, as obtained from (35):

$$\mathcal{H}_{11} = F_{H_1} \left(-\frac{\sqrt{15}}{4\sqrt{7}}Q_{H\theta} + \frac{5}{4\sqrt{7}}Q_{H\epsilon} \right) + F_{H_2} \left(\frac{\sqrt{5}}{16\sqrt{7}}Q_{H\theta} + \frac{3\sqrt{3}}{16\sqrt{7}}Q_{H\epsilon} \right) \quad (41)$$

By confronting (40) and (41) it is seen that the special coupling case dictates a relationship between the two JT force-elements in h -space:

$$\begin{aligned} F_{H_1} &= \frac{1}{2\sqrt{7}}k_{T_1} \\ F_{H_2} &= -\frac{3\sqrt{3}}{2\sqrt{7}}k_{T_1} \end{aligned} \quad (42)$$

The Hamiltonian for the $T_1 \times \Gamma_7$ coupling case can thus be projected onto the general Hamiltonian in the following way:

$$\begin{aligned} \mathcal{H}(T_1 \times h) &= k_{T_1} \left[\frac{1}{2\sqrt{7}}\mathcal{H}_1/F_{H_1} - \frac{3\sqrt{3}}{2\sqrt{7}}\mathcal{H}_2/F_{H_2} \right] \\ &= |k_{T_1}| [\cos \omega \times \mathcal{H}_1/F_{H_1} + \sin \omega \times \mathcal{H}_2/F_{H_2}] \end{aligned} \quad (43)$$

with $\tan \omega = -3\sqrt{3}$. Notice that the operator part in brackets is fully normalised.

Table 9. $T_2 \otimes \Gamma_6 = \Gamma_9$

T_2	Γ_6	Γ_9					
		$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$-\frac{5}{2}$
0	α	$\frac{1}{2\sqrt{2}}$	\cdot	$\frac{1}{2}$	\cdot	$\frac{\sqrt{5}}{2\sqrt{2}}$	\cdot
0	β	\cdot	$\frac{-\sqrt{5}}{2\sqrt{2}}$	\cdot	$\frac{-1}{2}$	\cdot	$\frac{-1}{2\sqrt{2}}$
1	α	\cdot	$\frac{-1}{4}$	\cdot	$\frac{\sqrt{5}}{2\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{4}$
1	β	$\frac{3}{4}$	\cdot	$\frac{1}{2\sqrt{2}}$	\cdot	$\frac{-\sqrt{5}}{4}$	\cdot
-1	α	\cdot	$\frac{\sqrt{5}}{4}$	\cdot	$\frac{-1}{2\sqrt{2}}$	\cdot	$\frac{-3}{4}$
-1	β	$\frac{\sqrt{5}}{4}$	\cdot	$\frac{-\sqrt{5}}{2\sqrt{2}}$	\cdot	$\frac{1}{4}$	\cdot

An entirely similar treatment can be made for the $T_2 \times \Gamma_6$ coupling case, using the coefficients in Table 9 and the Hamiltonian in (38). This yields:

$$\begin{aligned}
 F_{H_1} &= \frac{2}{\sqrt{7}} k_{T_2} \\
 F_{H_2} &= \frac{\sqrt{3}}{\sqrt{7}} k_{T_2}
 \end{aligned} \tag{44}$$

which also corresponds to a normalised operator with $\tan \omega = \sqrt{3}/2$. In both these special coupling cases the $\Gamma_9 \times h$ Hamiltonians have spherical symmetry due to the spherical invariance of the underlying $T \times h$ Hamiltonians.

7 Conclusion

This paper was devoted to a rigorous derivation of the icosahedral coupling coefficients for the $\Gamma_9 \times (g \oplus 2h)$ Jahn-Teller problem, using available spin-orbit coupling coefficients. Special attention was given to the treatment of the time-reversal operator, which gives rise to the symplectic form of the resulting Hamiltonian. The particular group theoretical property that the sextet level can be generated by direct multiplication of an orbital triplet with a doublet of pseudospin was shown to give rise to special coupling cases. The main symmetry breaking mechanisms enclosed in this Hamiltonian are described elsewhere [1]. Further studies are needed to analyse the parent symplectic structure of this interesting JT problem, and determine its dynamical features.

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