Irreducible Tensor Bases for the Frobenius Algebra of a Finite Unitary Group

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Symmetry adaptation to a finite group is often accomplished by projection with operators that are elements of a matric basis of the Frobenius algebra of the group. The matric basis elements are expressed in terms of the regular, or group, basis of the algebra by means of the irreducible representations. It is shown here for a unitary group that this algebra is also spanned by an irreducible tensor basis expressed on the matric basis with coupling coefficients. The centrum of the algebra is spanned by the invariant elements of this basis. Another irreducible tensor basis is obtained by completely reducing the representation of the group generated by similarity transforming itself. This conjugacy representation is partially reduced by the conjugacy classes so that each of the tensor basis elements is a linear combination of elements from a given class. The relation between this basis and the previous one is discussed. An example is provided for the point group C_{3v} isomorphic to the symmetric group $S(3)$.

I. INTRODUCTION

Algebras of finite groups—Frobenius algebras—are important in the quantum mechanical treatment of systems with finite symmetry groups such as molecular structures or collections of spins.[1,2] The Heisenberg exchange Hamiltonian, for example, is an element of the group algebra of the symmetric group of permutations.[3–5] Symmetry adaptation, constructing a basis transforming under the group according to a completely reduced representation, is facilitated with operators that are matric basis elements of the algebra. Symmetry adaptation may be the most common application of Frobenius group algebra.

A special case of symmetry adaptation is the construction of algebraic invariants that do not change under transformation by elements of the group. Of particular interest are invariants in the Frobenius group algebra itself. Strictly invariant algebraic elements that commute with every element of the algebra constitute the algebra's centrum or kernel.

The generalization of invariants is irreducible tensorial sets:[1,6–8]

$$\{t_r^\alpha, r = 1, 2, ..., f(\alpha)\} \tag{1.1}$$

whose elements transform irreducibly under elements of G:

$$G_a t_r^\alpha G_a^{-1} = \sum_{r'}^{f(\alpha)} [G_a]_{r'r}^\alpha t_{r'}^\alpha \tag{1.2}$$

where $f(\alpha)$ is the dimension of the Γ^α irreducible representation. For the invariant case, $f(A) = 1$ and $[G_a]_{11}^A = 1$. In previous work, normalized irreducible tensorial matric bases of matrix spaces have been exploited in various applications. In this paper, two irreducible tensor bases are constructed for a group algebra. These bases exhibit a decomposition of the algebra into invariant subspaces that, except for the centrum, are not algebras. Relations between the various bases are considered.

In sections II and III algebraic concepts are reviewed for the regular and matric bases. A general algorithm for symmetry adpatation is considered in section IV, and an irreducible tensor basis obtained from the matric basis is presented in section V. In section VI an alternative irredudible tensor basis is obtained from the conjugacy representation on the regular basis. Finally, in section VII the subalgebra spanned by the invariant irreducible tensors is related to the center of the algebra. The point group C_{3v} isomorphic to the symmetric group $S(4)$, is used as an example.

II. FROBENIUS ALGEBRA: REGULAR BASIS

A finite group, G, is denoted here by the ordered set:

$$G = \{G_1, G_2, ..., G_g\} \tag{2.1}$$

where G_1 is taken to be the identity. It is convenient to indicate the inverse of G_a by $G_{\bar{a}}$. The regular representation, Γ^R, of G consists of the set of $g \times g$ permutation matrices generated according to

$$G_a G = G[G_a]^R \tag{2.2}$$

The Frobenius, or finite group, algebra of G is $A(G)$ with a regular basis isomorphic to G. In the present context any distinction between G and the regular basis of $A(G)$ is unimportant. The elements $X \in A(G)$ are written

$$X = \sum_a^g (X)_a G_a \tag{2.3}$$

The structure constants of the regular basis are defined by

$$G_a G_b = \sum_c^g \gamma(ab;c) G_c \tag{2.4}$$

so that

$$\gamma(ab;c) = \begin{cases} 1, & \text{if } G_a G_b = G_c \\ 0, & \text{otherwise} \end{cases} \tag{2.5}$$

Comparison of (2.4) with (2.3) reveals that the structure constants are expressed in terms of expansion coefficients according to $\gamma(ab;c) = (G_a G_b)_c$. Comparison with (2.2) further demonstrates that the structure constants are related to the matrix elements of the regular representation by $\gamma(ab;c) = [G_a]_{cb}^R$, so that $(G_a G_b)_c = [G_a]_{cb}^R$.

Since only the identity has nonzero elements on the diagonal of the regular representation, it follows that the trace of each matrix $[G_a]^R$ is zero except for $[G_1]^R$ which has a trace equal to g. Then the regular basis is orthogonal, but not normalized, with respect to the Cartesian inner product:

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$$\sum_a^g \sum_b^g ([X]^R_{ab})^* [Y]^R_{ab} = \mathrm{trace}([X]^{R\dagger}[Y]^R) \quad (2.6)$$

$$= g \sum_a^g (X)^*_a (Y)_a \quad (2.7)$$

III. MATRIC BASES

A finite group algebra is semisimple, that is, an orthogonal sum of simple matric subalgebras:[2]

$$A(G) = \sum_\alpha^M \oplus A^\alpha \quad (3.1)$$

where M is the number of nonequivalent irreducible representations as well as the number of conjugacy classes of G. As a result, $A(G)$ is spanned by a matric basis:

$$\{e^\alpha_{rs}, \alpha = 1, ..., M; r, s = 1, ..., f(\alpha)\} \quad (3.2)$$

where

$$e^\alpha_{rs} e^\beta_{tu} = \delta(\alpha,\beta)\, \delta(\mathrm{s,t}) e^\alpha_{ru} \quad (3.3)$$

Since both bases must have the same number of elements, the familiar relation

$$\sum_\alpha^M f(\alpha)^2 = g \quad (3.4)$$

follows immediately. Elements $X \in A(G)$ are expressed on the matric basis according to

$$X = \sum_\alpha^M \sum_r^{f(\alpha)} \sum_s^{f(\alpha)} [X]^\alpha_{rs} e^\alpha_{rs} \quad (3.5)$$

where, by (3.3),

$$[XY]^\alpha_{rs} = \sum_t^{f(\alpha)} [X]^\alpha_{rt} [Y]^\alpha_{tu} \quad (3.6)$$

In particular, the expansion coefficients of the regular basis on the matric basis are the irreducible representations of G:

$$G_a = \sum_\alpha^M \sum_r^{f(\alpha)} \sum_s^{f(\alpha)} [G_a]^\alpha_{rs} e^\alpha_{rs} \quad (3.7)$$

Inversion of this relation with the help of (2.6) yields

$$e^\alpha_{rs} = \frac{f(\alpha)}{g} \sum_a^g [G_a]^\alpha_{sr} G_a \quad (3.8)$$

The familiar orthogonality relations on the irreducible representations follow immediately from (3.7) and (3.8). The matric basis elements transform under the regular basis elements according to

$$G_a e^\alpha_{rs} = \sum_{r'}^{f(\alpha)} [G_a]^\alpha_{r'r} e^\alpha_{r'r} \quad (3.9)$$

$$e^\alpha_{rs} G_a = \sum_{s'}^{f(\alpha)} [G_a]^\alpha_{ss'} e^\alpha_{rs'} \quad (3.10)$$

These properties justify the use of matric basis elements as symmetry projectors and transfer operators. The matric basis elements are orthogonal with respect to the Cartesian inner product:

$$\mathrm{trace}\{[e^\alpha_{rs}]^{R\dagger}[e^{\alpha'}_{r's'}]^R\} = \delta(\alpha,\alpha')\, \delta(r,r')\, \delta(s,s')\, f(\alpha) \quad (3.11)$$

A multiplication table, a set of irreducible representations, and a character table for C_{3v} are given in Tables I–III. Corresponding matric basis elements are displayed in Table IV.

Table I. Multiplication Table for the Point Group C_{3v}[a]

I	σ_{1v}	σ_{2v}	σ_{3v}	C_3	C_3^2
σ_{1v}	I	C_3	C_3^2	σ_{2v}	σ_{3v}
σ_{2v}	C_3^2	I	C_3	σ_{3v}	σ_{1v}
σ_{3v}	C_3	C_3^2	I	σ_{1v}	σ_{2v}
C_3	σ_{3v}	σ_{1v}	σ_{2v}	C_3^2	I
C_3^2	σ_{2v}	σ_{3v}	σ_{1v}	I	C_3

[a] The σ are reflections, and the C_3 are rotations.

Table II. Irreducible Representations for C_{3v}[a]

	I	σ_{1v}	σ_{2v}	σ_{3v}	C_3	C_3^2
A_1	[1]	[1]	[1]	[1]	[1]	[1]
A_2	[1]	[−1]	[−1]	[−1]	[1]	[1]
E	$\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$	$\begin{bmatrix}-a & -b\\-b & a\end{bmatrix}$	$\begin{bmatrix}-a & b\\b & a\end{bmatrix}$	$\begin{bmatrix}-a & -b\\b & -a\end{bmatrix}$	$\begin{bmatrix}-a & b\\-b & -a\end{bmatrix}$

[a] $a = 1/2$; $b = 3^{1/2}/2$.

Table III. Character Table for C_{3v}

	I	$\sigma_{1v}, \sigma_{2v}, \sigma_{3v}$	C_3, C_3^2
A_1	1	1	1
A_2	1	−1	1
E	2	0	−1

Table IV. Matric Basis Elements for the Frobenius Algebra of C_{3v} Constructed from the Irreducible Representations in Table II

$$e^{A_1}_{11} = {}^1/_6(I + \sigma_{1v} + \sigma_{2v} + \sigma_{3v} + C_3 + C_3^2)$$
$$e^{A_2}_{11} = {}^1/_6(I - \sigma_{1v} - \sigma_{2v} - \sigma_{3v} + C_3 + C_3^2)$$
$$e^{E}_{11} = {}^1/_3\{I + \sigma_{1v} - {}^1/_2(\sigma_{2v} + \sigma_{3v} + C_3 + C_3^2)\}$$
$$e^{E}_{12} = (1/2(3^{1/2}))(-\sigma_{2v} + \sigma_{3v} - C_3 + C_3^2)$$
$$e^{E}_{21} = (1/2(3^{1/2}))(-\sigma_{2v} + \sigma_{3v} + C_3 - C_3^2)$$
$$e^{E}_{22} = {}^1/_3\{I - \sigma_{1v} + {}^1/_2(\sigma_{2v} + \sigma_{3v} - C_3 - C_3^2)\}$$

IV. SYMMETRY ADAPTATION

Let a basis, $B(\omega)$, for a vector space $V(\omega)$ invariant under G be

$$B(\omega) = \{|\omega i\rangle, i = 1, ..., f(\omega)\} \quad (4.1)$$

and let it generate a matrix representation Γ^ω of the group G by

$$G_a B(\omega) = B(\omega)[G_a]^\omega \quad (4.2)$$

Then $B(\omega)$ can be symmetry adapted according to the following algorithm:[1]

A. Generate the matrix representations, $[e^\alpha_{rs}]^\omega$, of the matric basis elements on $B(\omega)$ by using eq 3.8.

$$[e^\alpha_{rs}]^\omega = \frac{f(\alpha)}{g} \sum_a^g [G_a]^\alpha_{sr} [G_a]^\omega \quad (4.3)$$

B. For each α such that trace $[e^\alpha_{11}]^\omega \neq 0$, obtain the eigenvector with eigenvalue 1 of the hermitian idempotent matrices $[e^\alpha_{11}]^\omega$. These may be denoted

$$\{|\omega;\rho\alpha 1\rangle, \rho = 1, ..., f(\omega;\alpha)\} \quad (4.4)$$

Table V. Reduction of Kronecker Products of Irreducible Representations of C_{3v}

	A_1	A_2	E
A_1	A_1	A_2	E
A_2	A_2	A_1	E
E	E	E	$A_1 + A_2 + E$

Table VI. Coupling Coefficients for the $\Gamma^E \times \Gamma^E$ Kronecker Product

$E \times E$	A_1	A_2	$E1$	$E2$
$E1,E1$	$1/2^{1/2}$	0	$-1/2^{1/2}$	0
$E1,E2$	0	$1/2^{1/2}$	0	$1/2^{1/2}$
$E2,E1$	0	$-1/2^{1/2}$	0	$1/2^{1/2}$
$E2,E2$	$1/2^{1/2}$	0	$1/2^{1/2}$	0

such that

$$e^{\alpha}_{11}|\omega;\rho\alpha 1\rangle = |\omega;\rho\alpha 1\rangle \tag{4.5}$$

C. Obtain the remaining symmetry-adapted vectors by the operations

$$|\omega;\rho\alpha r\rangle = e^{\alpha}_{r1}|\omega;\rho\alpha 1\rangle \tag{4.6}$$

Since $[e^{\alpha}_{11}]^{\omega}$ is hermitian, the transformation to the symmetry-adapted basis is unitary and can be written

$$|\omega;\rho\alpha r\rangle = \sum_{i}^{f(\omega)} |\omega i\rangle\langle\omega i|\rho\alpha r\rangle \tag{4.7}$$

The matrix representations of the matric basis elements are given in terms of the transformation coefficients by

$$[e^{\alpha}_{rs}]^{\omega}_{ij} = \sum_{\rho}^{f(\omega;\alpha)} \langle\omega i|\rho\alpha r\rangle\langle\rho\alpha s|\omega j\rangle \tag{4.8}$$

The unitary transformation coefficients which reduce the Kronecker product representation $\Gamma^{\alpha_1} \times \Gamma^{\alpha_2}$ are the coupling coefficients:

$$|\alpha_1,\alpha_2;\rho\alpha r\rangle = \sum_{r_1}^{f(\alpha_1)}\sum_{r_2}^{f(\alpha_2)} |\alpha_1 r_1\rangle|\alpha_2 r_2\rangle\langle\alpha_1 r_1,\alpha_2 r_2|\rho\alpha r\rangle \tag{4.9}$$

In this case the representations of the matric basis elements are given by

$$[e^{\alpha}_{rs}]^{\alpha_1\alpha_2}_{(r_1r_2)(s_1s_2)} = \frac{f(\alpha)}{g}\sum_{a}^{g}[G_a]^{\alpha}_{sr}[G_a]^{\alpha_1}_{r_1s_1}[G_a]^{\alpha_2}_{r_2s_2}$$

$$= \sum_{\rho}^{f(\alpha_1\alpha_2;\alpha)} \langle\alpha_1 r_1\alpha_2 r_2|\rho\alpha r\rangle\langle\rho\alpha s|\alpha_1 s_1\alpha_2 s_2\rangle \tag{4.10}$$

For simply reducible groups, the frequencies $f(\alpha_1\alpha_2;\alpha)$ are zero or one for all α_1, α_2, and α, and the last expression in (4.10) is either a simple product or zero. Reduction of the Kronecker products of irreducible representations of C_{3v} are indicated in Table V, and coupling coefficients that reduce $\Gamma^E \times \Gamma^E$ are given in Table VI.

V. IRREDUCIBLE TENSOR BASIS

The elements of a matric basis (3.2) of $A(G)$ transform as tensor operators under G. Combining (3.9) and (3.10) gives

$$G_a e^{\alpha}_{rs} G_{\bar{a}} = \sum_{r'}^{f(\alpha)}\sum_{s'}^{f(\alpha)} [G_a]^{\alpha}_{r'r}[G_{\bar{a}}]^{\alpha}_{ss'}e^{\alpha}_{r's'}$$

$$= \sum_{r'}^{f(\alpha)}\sum_{s'}^{f(\alpha)} [G_a]^{\alpha}_{r'r}([G_a]^{\alpha}_{s's})^{*}e^{\alpha}_{r's'} \tag{5.1}$$

where the second equality follows from the unitary property. Then the matric basis elements e^{α}_{rs} transform according to the Kronecker product representation $\Gamma^{\alpha} \times \Gamma^{\hat{\alpha}}$, where $\hat{\alpha}$ indicates the representation contragredient to Γ^{α}. The irreducible tensor basis elements are then obtained by transforming with the coupling coefficients

$$n^{\alpha;\rho\beta}_{t} = \sum_{r}^{f(\alpha)}\sum_{s}^{f(\alpha)} e^{\alpha}_{rs}\langle\alpha r,\hat{\alpha}s|\rho\beta t\rangle \tag{5.2}$$

with $\rho = 1, 2, ..., f(\alpha,\alpha;\beta)$. Irreducible tensor basis elements for C_{3v} are given in Table VII. As in (1.2), these operators transform irreducibly under elements of G:

$$G_a n^{\alpha;\sigma\beta}_{t} G_{\bar{a}} = \sum_{t'}^{f(\beta)} [G_a]^{\beta}_{t't}\, n^{\alpha;\sigma\beta}_{t'} \tag{5.3}$$

These irreducible tensors are orthogonal with respect to the Cartesian inner product:

$$\mathrm{trace}\{[n^{\alpha;\sigma\beta}_{t}]^{R\dagger}\,[n^{\alpha';\sigma'\beta'}_{t'}]^{R} = \delta(\alpha,\alpha')\,\delta(\sigma,\sigma')\,\delta(\beta,\beta')\,\delta(t,t')\,f(\alpha) \tag{5.4}$$

For the special invariant case $\beta = A$, (5.2) reduces to

$$n^{\alpha;A}_{1} = \frac{1}{[f(\alpha)]^{1/2}}\sum_{r}^{f(\alpha)} e^{\alpha}_{rr}$$

$$= \frac{1}{[f(\alpha)]^{1/2}}e^{\alpha} \tag{5.5}$$

where the simple matric projector, e^{α}, is the modulus for A^{α} of (3.1). Each simple matric algebra A^{α} is spanned by $f(\alpha)^2$ irreducible tensors $n^{\alpha;\rho\beta}_{t}$, with the invariant A tensor occurring once.

For simply reducible groups the usual coupling coefficients can be used in (5.2).[1,9,10] The unnecessary frequency index ρ is dropped, and it can be shown from (4.10) that the coupling coefficients for Γ^{β} in $\Gamma^{\alpha} \times \Gamma^{\hat{\alpha}}$ can be related to those for Γ^{α} in $\Gamma^{\beta} \times \Gamma^{\alpha}$ by

$$\langle\alpha r\hat{\alpha}s|\beta t\rangle = \frac{[f(\beta)]^{1/2}}{[f(\alpha)]^{1/2}}\langle\beta t\alpha s|\alpha r\rangle^{*}$$

$$= \frac{[f(\beta)]^{1/2}}{[f(\alpha)]^{1/2}}\langle\alpha r|\beta t\alpha s\rangle \tag{5.6}$$

With an appropriate phase choice, ϕ, the coupling coefficient $\langle\alpha r|\beta t\alpha s\rangle$ divided by $[f(\alpha)]^{1/2}$ is a "3α" symbol, or V coefficient as defined by Griffith, analogous to the $3-j$ symbol of SU(2).[7] With this notation, (5.2) can be written for simply reducible groups as

$$n^{\alpha;\beta}_{t} = \sum_{r}^{f(\alpha)}\sum_{s}^{f(\alpha)} e^{\alpha}_{rs}[f(\alpha)]^{1/2}\phi V\begin{pmatrix}\alpha & \beta & \alpha\\ \hat{r} & t & s\end{pmatrix} \tag{5.7}$$

where $\hat{r}$ indicates the appropriate contragredient index and ϕ is the phase factor. The matric basis coefficients for these

Table VII. Normalized Irreducible Tensor Operators in Terms of Matric Basis Elements Using the Coupling Coefficients of Table VI

$$n_1^{A_1;A_1} = e_{11}^{A_1}$$
$$n_1^{A_2;A_1} = e_{11}^{A_2}$$
$$n_1^{E;A_1} = (1/2^{1/2})(e_{11}^E + e_{22}^E)$$
$$n_1^{E;A_2} = (1/2^{1/2})(e_{12}^E - e_{21}^E)$$
$$n_1^{E;E} = (-1/2^{1/2})(e_{11}^E - e_{22}^E)$$
$$n_2^{E;E} = (1/2^{1/2})(e_{12}^E + e_{21}^E)$$

operators are then

$$[n_t^{\alpha;\beta}]_{rs}^{\alpha} = [f(\alpha)]^{1/2}\phi V\begin{pmatrix} \alpha & \beta & \alpha \\ r & t & s \end{pmatrix} \tag{5.8}$$

identical to the elements of normalized irreducible tensorial matrices and consistent with the Wigner–Eckart theorem.[1] A basis of normalized irreducible tensorial operators for C_{3v} is displayed in Table VII.

For simply reducible groups, the irreducible tensor operators multiply according to

$$n_{t_1}^{\alpha;\beta_1} n_{t_2}^{\alpha';\beta_2} = \delta(\alpha,\alpha') \sum_{\beta_3} \sum_{t_3}^{f(\beta_3)} \gamma(\alpha,\beta_1,\alpha,\beta_2,\alpha,\beta_3;t_1,t_2,t_3) n_{t_3}^{\alpha;\beta_3} \tag{5.9}$$

with structure constants given by

$$\gamma(\alpha,\beta_1,\alpha,\beta_2,\alpha,\beta_3;\, t_1,t_2,t_3) = \phi[f(\beta_1)\, f(\beta_2)\, f(\beta_3)]^{1/2}\, W\begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \\ \alpha & \alpha & \alpha \end{pmatrix} V\begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \\ t_1 & t_2 & t_3 \end{pmatrix} \tag{5.10}$$

where the W coefficient, as defined by Griffith, is analogous to the $6\text{-}j$ symbol of SU(2).[7] The first sum is over all β_3 such that the coupling frequencies $f(\beta_1,\beta_2;\beta_3)$ are not zero.

Therefore the set of irreducible tensors

$$\{n_t^{\alpha;\beta},\, t = 1, 2, ..., f(\beta)\} \tag{5.11}$$

spans a subspace of A^α invariant under the equivalence transformation (5.3), but is not, in general, closed under multiplication. From (5.10) only the invariant $\beta = A$ tensors multiply to give A tensors. As discussed below, these invariant tensors span the centrum which is indeed a subalgebra.

Using the unitary property of coupling coefficients, the matric basis elements are expressed in terms of the irreducible tensors according to

$$e_{rs}^{\alpha} = \sum_{\beta}^{M} \sum_{\sigma}^{f(\alpha,\alpha;\beta)} \sum_{t}^{f(\beta)} n_t^{\alpha;\sigma\beta} \langle \sigma\beta t | \alpha r, \hat{\alpha} s \rangle \tag{5.12}$$

and by substituting (5.12) in (3.7), the regular basis elements are expressed in terms of these tensors as

$$G_a = \sum_{\alpha}^{M} \sum_{r}^{f(\alpha)} \sum_{s}^{f(\alpha)} \sum_{\beta}^{M} \sum_{\sigma}^{f(\alpha,\alpha;\beta)} \sum_{t}^{f(\beta)} [G_a]_{rs}^{\alpha} \langle \sigma\beta t | \alpha r, \hat{\alpha} s \rangle n_t^{\alpha;\sigma\beta} \tag{5.13}$$

Note that (5.13) is a unitary transformation. The inverse to (5.13) is obtained by substituting (3.8) in (5.2):

$$n_t^{\alpha;\sigma\beta} = \frac{f(\alpha)}{g} \sum_{a}^{g} \sum_{r}^{f(\alpha)} \sum_{s}^{f(\alpha)} [G_a]_{sr}^{\alpha} \langle \alpha r, \hat{\alpha} s | \sigma\beta t \rangle G_a \tag{5.14}$$

VI. CONJUGACY REPRESENTATION

Analogous to the regular representation of G is the conjugacy representation, Γ^C, defined by

$$G_a G G_a^{-1} = G[G_a]^C \tag{6.1}$$

Conjugacy transformations for C_{3v} are given in Table VIII.

Table VIII. Conjugacy Transformations on Elements of C_{3v}: $G_a G_b G_a$

	b: I	σ_{1v}	σ_{2v}	σ_{3v}	C_3	C_3^2
I	I	σ_{1v}	σ_{2v}	σ_{3v}	C_3	C_3^2
σ_{1v}	I	σ_{1v}	σ_{3v}	σ_{2v}	C_3^2	C_3
σ_{2v}	I	σ_{3v}	σ_{2v}	σ_{1v}	C_3^2	C_3
σ_{3v}	I	σ_{2v}	σ_{1v}	σ_{3v}	C_3^2	C_3
C_3	I	σ_{2v}	σ_{3v}	σ_{1v}	C_3	C_3^2
C_3^2	I	σ_{3v}	σ_{1v}	σ_{2v}	C_3	C_3^2

Table IX. Irreducible Tensorial Operators for the Conjugacy Classes

$$q(I)_1^{A_1} = I$$
$$q(\sigma)_1^{A_1} = (1/3^{1/2})(\sigma_{1v} + \sigma_{2v} + \sigma_{3v})$$
$$q(\sigma)_1^{E} = (1/6^{1/2})(2\sigma_{1v} - \sigma_{2v} - \sigma_{3v})$$
$$q(\sigma)_2^{E} = (1/2^{1/2})(\sigma_{2v} - \sigma_{3v})$$
$$q(C)_1^{A_1} = (1/2^{1/2})(C_3 + C_3^2)$$
$$q(C)_1^{A_2} = (1/2^{1/2})(C_3 - C_3^2)$$

Since the conjugacy classes are invariant under the similarity transformation on the left of (6.1), Γ^C is partially reduced to a direct sum of permutation matrices. Complete reduction can be carried out by the symmetry adaptation methods of section IV, yielding an irreducible tensor basis for the algebra. Letting the τth conjugacy class with n_τ members be denoted C_τ, the general transformation is

$$q(\tau)_t^{\sigma\beta} = \sum_{a\in\tau}^{n_\tau} G_a \langle \tau;a | \sigma\beta t \rangle \tag{6.2}$$

It is convenient to take the coefficients $\langle \tau;a|\sigma\beta t\rangle$ to be zero if G_a does not belong to C_τ. Tensor elements of this sort for C_{3v} are displayed in Table IX.

The invariant $\beta = A$ tensor occurs once in each class and must in fact be proportional to the class operator K_τ, the simple sum of all elements in C_τ. Due to unitarity, the proportionality constant must be $1/n_\tau^{1/2}$:

$$q(\tau)_1^A = \frac{1}{n_\tau^{1/2}} \sum_{a\in\tau}^{n_\tau} G_a = \frac{1}{n_\tau^{1/2}} K_\tau \tag{6.3}$$

These operators are orthogonal with respect to the Cartesian inner product

$$\mathrm{trace}\{[q(\tau)_t^{\sigma\beta}]^{R\dagger}[q(\tau')_{t'}^{\sigma'\beta'}]^R\} = \delta(\tau,\tau')\,\delta(\sigma,\sigma')\,\delta(\beta,\beta')\,\delta(t,t')g \tag{6.4}$$

Elements, $n_t^{\alpha;\sigma\beta}$, of the irreducible tensor basis in section V belong to specific simple matric subalgebras: A^α. An irreducible tensor defined in this section, $q(\tau)_t^{\sigma\beta}$, is expressed in terms of elements from a single conjugacy class of G. The transformation between them is obtained by substituting (3.7) and (5.12) in (6.2):

$$q(\tau)_t^{\sigma\beta} = \sum_{a\in\tau}^{n_\tau} \sum_{\alpha}^{M} \sum_{r}^{f(\alpha)} \sum_{s}^{f(\alpha)} \sum_{\sigma'}^{f(\alpha,\alpha;\beta)} [G_a]_{rs}^{\alpha} \langle \tau;a|\sigma\beta t\rangle \langle \sigma'\beta t|\alpha r,\hat{\alpha} s\rangle n_t^{\alpha;\sigma'\beta} \tag{6.5}$$

This transformation is shown in Table X for C_{3v}. For the special case $\beta = A$, (6.5) reduces to

$$K_\tau = \sum_{\alpha}^{M} \frac{n_\tau}{f(\alpha)} \chi_\tau^\alpha e^\alpha \tag{6.6}$$

which is the familiar relation between elements of two traditional bases of the centrum.[11]

Table X. Conjugacy Class Irreducible Tensorial Operators Expressed in Terms of the Normalized Irreducible Tensorial Operators in Table VII

$$q(I)_1^{A_1} = n_1^{A_1;A_1} + n_1^{A_2;A_1} + 2^{1/2}n_1^{E;A_1}$$
$$q(\sigma)_1^{A_1} = 3^{1/2}n_1^{A_1;A_1} - 3^{1/2}n_1^{A_2;A_1}$$
$$q(\sigma)_1^{E} = -3^{1/2}n_1^{E;E}$$
$$q(\sigma)_2^{E} = -3^{1/2}n_2^{E;E}$$
$$q(C)_1^{A_1} = 2^{1/2}n_1^{A_1;A_1} + 2^{1/2}n_1^{A_2;A_1} - n_1^{E;A_1}$$
$$q(C)_1^{A_2} = 3^{1/2}n_1^{E;A_2}$$

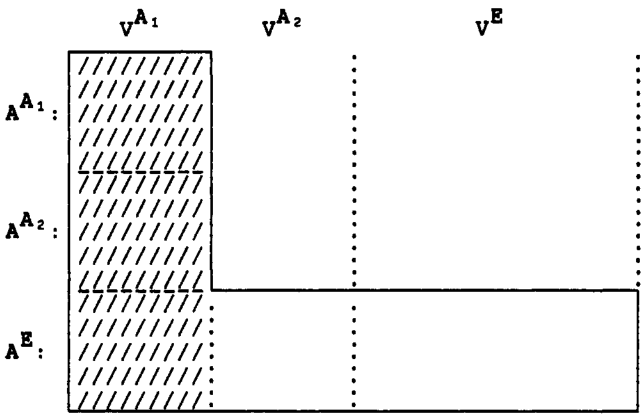

Figure 1. Representation of the structure of the Frobenius algebra of C_{3v}. Vertical divisions indicate the invariant subspaces spanned by the normalized irreducible tensorial operators. Shaded area is the centrum, the only subspace in this decomposition that is an algebra. Horizontal divisions represent the invariant subalgebras A^{α}.

VII. CONCLUSION

Irreducible tensorial bases exhibit structures for Frobenius algebras that are alternative to the conventional orthogonal decomposition by simple matric projectors. This is illustrated in Figure 1. The invariant subspaces spanned by tensor operators of the same species are not algebras except for the invariant elements. These structures are graphically illustrated for C_{3v} in Figure 1. The invariant tensors span the centrum of the algebra, giving in one case the simple matric projectors and in the other the class operators. It is anticipated that studies of subgroup and subclass relationships, as discussed by Wigner, will profit from the irreducible tensor treatment.[12]

The primary difficulty in applying the symmetry adaptation algorithm described in section IV is evaluating the matrices $[e^{\alpha}{}_{rs}]^{\omega}$ from eq 4.3. All the matrices of the representation Γ^{ω}, as well as the irreducible representations, are necessary. It may happen that the matrices representing the irreducible tensors, $[n_t^{\alpha;\sigma\beta}]^{\omega}$, are more easily obtained. Then the necessary matrices are given by the transformation

$$[e^{\alpha}_{rs}]^{\omega} = \sum_{\sigma}^{f(\alpha,\alpha;\beta)} \sum_{\beta}^{M} \sum_{t}^{f(\beta)} \langle \sigma\beta t|\alpha r,\hat{\alpha}s\rangle [n_t^{\alpha;\sigma\beta}]^{\omega} \qquad (7.1)$$

where the coupling coefficients can be expressed in terms of $3-\alpha$ symbols.

This work is an attempt to integrate into a consistent algebraic framework concepts that are usually treated separately. The Wigner–Eckart theorem has not generally been considered a group algebraic property, but the irreducible tensor basis demonstrates that the two are related.

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