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Finite Group Theory for Large Systems. 1. Symmetry-Adaptation

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The challenge of symmetry-adapting large basis sets to finite groups, apart from extensive calculations with large matrices, is obtaining linearly independent bases for frequently repeated irreducible representations, a process that is not determined by the group theory. The usual projection method is modified here to solve this problem efficiently and systematically. The resulting basis is suitably conditioned so that repeated irreducible representations are identical as required by the symmetry-generation theorem.

I. INTRODUCTION

The first in a series on the application of finite group theory to large systems, principally in quantum chemistry, this article addresses the problem of symmetry-adaptation—constructing bases of linear spaces that transform according to completely reduced representations of a finite group. The challenge of symmetry-adaptation, particularly for large dimensions, is obtaining the bases for repeated representations, solved in principle in an earlier algorithm by using orthogonal eigenvectors of an Hermitian projection operator matrix.[1,2] High degeneracies may lead to computational difficulties for large dimensions, however, and a modification to remedy this shortcoming based on the properties of Hermitian idempotent matrices is given here.

Finite groups play an important role in the study of molecules, crystals, and clusters in chemistry and materials science although applications have usually been restricted to small or moderately sized systems due to computational limitations.[3−7] To be practical for large systems, finite group theory requires both computer calculation and the advanced methods of irreducible tensorial sets including the Wigner-Eckart theorem and the symmetry generation theorem.[8−11] Since these methods depend on symmetry-adapted bases, the construction of such bases for large dimensions is particularly important.

An illustration of the algorithm described here is taken from the simple Hückel treatment of icosahedral fullerene, C_{60}. The defining basis for the state space is spanned by the 60 atomic p_z orbitals that generate a reducible representation of the icosahedral point group, $\mathscr{I}_h$. In the next article in this series, generating relations and irreducible representations for $\mathscr{I}_h$ are systematically constructed.[12] In the third article, these methods are employed to apply the symmetry-generation theorem to icosahedral fullerene, C_{60}.[13]

II. SYMMETRY-ADAPTED BASIS

A basis, $B(\omega)$, of a vector space, $V(\omega)$ is symmetry-adapted to a group G if all of its elements transform irreducibly under elements of G

$$G_a|\omega;\rho\alpha r\rangle = \sum_{r'=1}^{f(\alpha)} [G_a]^{\rho\alpha}_{r'r}|\omega;\rho\alpha r'\rangle \tag{2.1}$$

where $[G_a]^{\rho\alpha}_{r'r}$ is the r',r element of the matrix representing group operator G_a in the ρth occurrence of the αth irreducible representation, $\Gamma^\alpha(G)$, of G. The full basis is

$$B(\omega) = \{|\omega;\rho\alpha r\rangle, r = 1, ..., f(\alpha); \alpha = 1, ..., M; \rho = 1, ..., f(\omega;\alpha)\} \tag{2.2}$$

where ω indicates the overall vector space, α designates a particular irreducible representation of dimension $f(\alpha)$, r indexes partner elements belonging to the same irreducible representation, M is the number of nonequivalent irreducible representations (and classes), ρ distinguishes repeated irreducible representations, and $f(\omega;\alpha)$ is the number of times the αth irreducible representation occurs in the reducible representation $\Gamma(\omega)$, given by the usual character formula

$$f(\omega;\alpha) = \frac{1}{g}\sum_{\sigma=1}^{M} n_\sigma \chi^\alpha_{\bar\sigma}\chi^\omega_\sigma \tag{2.3}$$

where g is the order of the group, σ indexes the classes of G, n_σ is the number of elements in the σth class, $\chi^\alpha_{\bar\sigma}$ is the character of the inverse of the σth class in the αth irreducible representation, and χ^ω_σ is the character of the σth class in the ω reducible representation. On this basis the matrix representation of G is completely reduced:

$$[G_a]^\omega = \begin{bmatrix} [G_a]^{1\alpha} & & & & 0 \\ & [G_a]^{2\alpha} & & & \\ & & \cdots & & \\ & & & [G_a]^{1\beta} & \\ 0 & & & & [G_a]^{1\gamma} \end{bmatrix} \tag{2.4}$$

In general, repeated representations, $[G_a]^{\rho\alpha}$ and $[G_a]^{\rho'\alpha}$, need only be equivalent to satisfy the definition of a symmetry-adapted basis. The symmetry-generation theorem, however, requires all repeated representations to be identical:

$$[G_a]^{\rho\alpha} = [G_a]^\alpha, \rho = 1,2, ..., f(\omega;\alpha) \tag{2.5}$$

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A symmetry-adapted basis for which this is true is termed suitably conditioned, and the bases produced by the methods described here satisfy this condition.

The elements of a symmetry-adapted basis are orthogonal over α and r but not necessarily over ρ:

$$\langle \omega;\rho\alpha r|\omega;\rho'\alpha' r'\rangle = \delta(\alpha,\alpha')\delta(r,r')\langle \omega;\rho\alpha||\omega;\rho'\alpha\rangle \quad (2.6)$$

For operators, O, that commute with the group:

$$[O,G] = 0 \quad (2.7)$$

matrix elements on the symmetry-adapted basis satisfy:

$$\langle \omega;\rho\alpha r|O|\omega;\rho'\alpha' r'\rangle = \delta(\alpha,\alpha')\delta(r,r')\langle \omega;\rho\alpha||O||\omega;\rho'\alpha\rangle \quad (2.8)$$

where $\langle \omega;\rho\alpha||O||\omega;\rho'\alpha\rangle$ is termed a reduced matrix element.

III. SYMMETRY-ADAPTATION

A vector space $V(\omega)$, of dimension $f(\omega)$ and invariant to a group G, is spanned by a defining basis $B(\omega)$

$$V(\omega){:}B(\omega) = \{|\omega i\rangle, i = 1, ..., f(\omega)\} \quad (3.1)$$

which generates a reducible unitary representation $\Gamma^{\omega}(G)$ of G according to

$$G_a|\omega i\rangle = \sum_{j}^{f(\omega)} [G_a]^{\omega}_{ji}|\omega j\rangle \quad (3.2)$$

Symmetry-adaptation by projection uses elements of the group algebra, specifically, the matric basis elements, or Wigner operators, given by[2]

$$e^{\alpha}_{rs} = \frac{f(\alpha)}{g}\sum_{a=1}^{g}[G_a^{-1}]^{\alpha}_{sr}G_a \quad (3.3)$$

where $[G_a^{-1}]^{\alpha}_{sr}$ is a matrix element of the irreducible representation $\Gamma^{\alpha}(G)$. Some key properties of these operators are summarized here.

For unitary groups, the Hermitian adjoints of these operators are

$$e^{\alpha\dagger}_{rs} = e^{\alpha}_{sr} \quad (3.4)$$

and they multiply according to

$$e^{\alpha}_{rs}\cdot e^{\beta}_{tu} = \delta(\alpha,\beta)\delta(s,t)e^{\alpha}_{ru} \quad (3.5)$$

The operators transform under the group elements according to the irreducible representations:

$$G_a e^{\alpha}_{rs} = \sum_{r'}^{f(\alpha)}[G_a]^{\alpha}_{r'r}\, e^{\alpha}_{r's} \quad (3.6)$$

The self-adjoint e^{α}_{rr} are idempotent

$$e^{\alpha}_{rr}\, e^{\alpha}_{rr} = e^{\alpha}_{rr} \quad (3.7)$$

and can function as projection operators. Other possible projectors are the idempotents

$$e^{\alpha} \equiv \sum_{r=1}^{f(\alpha)} e^{\alpha}_{rr} \quad (3.8)$$

which are also orthogonal:

$$e^{\alpha}\cdot e^{\beta} = \delta(\alpha,\beta)e^{\alpha} \quad (3.9)$$

The e^{α} can be expressed in terms of the group characters. The various idempotents sum to the identity:

$$I = \sum_{\alpha=1}^{M} e^{\alpha} = \sum_{\alpha=1}^{M}\sum_{r=1}^{f(\alpha)} e^{\alpha}_{rr} \quad (3.10)$$

Given a vector $|\omega;\rho\alpha 1\rangle$, such that

$$e^{\alpha}_{11}|\omega;\rho\alpha 1\rangle = |\omega;\rho\alpha 1\rangle \quad (3.11)$$

it follows from (3.5) that the remaining partners of $|\omega;\rho\alpha 1\rangle$ are obtained by

$$|\omega;\rho\alpha r\rangle = e^{\alpha}_{r1}|\omega;\rho\alpha 1\rangle \quad (3.12)$$

With (3.6), this ensures that the symmetry-adapted basis is suitably conditioned.

The matrices representing the e^{α}_{rs} on $B(\omega)$ are constructed by substituting the group matrix representations from (3.2) into (3.3):

$$[e^{\alpha}_{rs}]^{\omega}_{ij} = \frac{f(\alpha)}{g}\sum_{a=1}^{g}[G_a^{-1}]^{\alpha}_{sr}[G_a]^{\omega}_{ij} \quad (3.13)$$

Unless the Hermitian idempotent matrix $[e^{\alpha}_{11}]^{\omega}$ is the identity, its determinant is zero and its trace is $f(\omega;\alpha)$. It has $f(\omega;\alpha)$ eigenvectors with eigenvalue one and $f(\omega) - f(\omega;\alpha)$ eigenvectors with eigenvalue zero. Its rank is $f(\omega;\alpha)$, i.e., the size of the largest nonzero determinant obtainable from elements of $[e^{\alpha}_{11}]^{\omega}$ is $f(\omega;\alpha)$.

It follows that symmetry-adaptation is accomplished by determining the coefficients $\langle \omega i|\rho\alpha 1\rangle$ that give $f(\omega;\alpha)$ linearly independent eigenvectors to $[e^{\alpha}_{11}]^{\omega}$ with eigenvalue one

$$\{|\omega;\rho\alpha 1\rangle, \rho = 1, ..., f(\omega;\alpha)\} \quad (3.14)$$

for each occurring irreducible representation $\Gamma^{\alpha}(G)$. Orthonormal eigenvectors of $[e^{\alpha}_{11}]^{\omega}$ can in principle be obtained by any of the usual eigenvalue/eigenvector algorithms in which case the complete symmetry-adaptation transformation is unitary:

$$|\omega;\rho\alpha r\rangle = \sum_{i}^{f(\omega)}|\omega i\rangle\langle \omega i|\rho\alpha r\rangle \quad (3.15)$$

In this case, the symmetry-adapted basis is orthonormal only if the defining basis is orthonormal. Computational problems can arise for large matrices with high degeneracies due to precision limitations, however.

Alternatively, the direct projection method of symmetry-adaptation is to take f($\omega;\alpha$) linearly independent vectors of the form $e^{\alpha}_{11}|\omega i\rangle$ to be, after normalization, the $|\omega;\rho\alpha 1\rangle$. In effect, this means using $f(\omega;\alpha)$ linearly independent columns of $[e^{\alpha}_{11}]^{\omega}$. Linear independence is difficult to ensure for large dimensions, however, particularly when the projections are not orthogonal. A method for dealing with this is given in the next section.

IV. OBTAINING LINEARLY INDEPENDENT PROJECTIONS

Since $[e^{\alpha}_{11}]^{\omega}$ is idempotent and Hermitian, the matrix product of $[e^{\alpha}_{11}]^{\omega}$ times itself gives

$$
\begin{aligned}
[e^{\alpha}_{11}]^{\omega}_{ik} &= \sum_{j=1}^{f(\omega)} [e^{\alpha}_{11}]^{\omega}_{ij} [e^{\alpha}_{11}]^{\omega}_{jk} \\
&= \sum_{j=1}^{f(\omega)} [e^{\alpha}_{11}]^{\omega *}_{ji} [e^{\alpha}_{11}]^{\omega}_{jk} \qquad (4.1)
\end{aligned}
$$

so that the number $[e^{\alpha}_{11}]^{\omega}_{ik}$ is the Hermitian inner product of the ith and kth columns of $[e^{\alpha}_{11}]^{\omega}$, while $[e^{\alpha}_{11}]^{\omega}_{ii}$ is the norm squared of the ith column. Since the rank of $[e^{\alpha}_{11}]^{\omega}$ is $f(\omega;\alpha)$, a linearly independent set of this many columns of $[e^{\alpha}_{11}]^{\omega}$ can be assembled. The ith and kth columns of $[e^{\alpha}_{11}]^{\omega}$ are orthogonal if $[e^{\alpha}_{11}]^{\omega}_{ik}$ is zero and a mutually orthogonal set is linearly independent.

Generally, the best approach is to progressively assemble the set of projections by selecting columns of $[e^{\alpha}_{11}]^{\omega}$, setting up the matrix $[M]$ of mutual inner products of these columns from the elements of $[e^{\alpha}_{11}]^{\omega}$, and evaluating the determinant of $[M]$. If the absolute value of the determinant of $[M]$ is sufficiently large, the set is linearly independent. This set of vectors can be used as a nonorthogonal symmetry-adapted basis and can be normalized by dividing by the square root of the appropriate diagonal elements of $[e^{\alpha}_{11}]^{\omega}$.

If the inner product matrix, $[M]$, can be diagonalized, the basis transformation can be made unitary by using the eigenvectors of $[M]$. Normalization follows upon division by the square roots of corresponding eigenvalues.

In summary, the algorithm for different frequencies is as follows: $\boldsymbol{f(\omega;\alpha) = 0}$, $\Gamma(\alpha)$ does not occur in the reduced representation. $\boldsymbol{f(\omega;\alpha) = 1}$, the $\rho = 1$ projection is

$$
|\omega;1\alpha 1\rangle = e^{\alpha}_{11}|\omega i\rangle \Big/ \sqrt{[e^{\alpha}_{11}]^{\omega}_{ii}} \qquad (4.2)
$$

where i corresponds to any nonzero column of $[e^{\alpha}_{11}]^{\omega}$. The coefficients from (4.2) are

$$
\langle \omega j|1\alpha 1\rangle = [e^{\alpha}_{11}]^{\omega}_{ji} \Big/ \sqrt{[e^{\alpha}_{11}]^{\omega}_{ii}} \qquad (4.3)
$$

and

$$
\langle \omega j|1\alpha r\rangle = [e^{\alpha}_{r1}]^{\omega}_{ji} \Big/ \sqrt{[e^{\alpha}_{11}]^{\omega}_{ii}} \qquad (4.4)
$$

$\boldsymbol{f(\omega;\alpha) > 1}$**:**

1. Select $f(\omega;\alpha)$ linearly independent columns of $[e^{\alpha}_{11}]^{\omega}$ using as much of the upper left portion of $[e^{\alpha}_{11}]^{\omega}$ as necessary, ensuring that the matrix, $[M]$, is nonsingular.

2. Obtain the $f(\omega;\alpha)$ eigenvalues, $E(\rho)$, and corresponding eigenvectors, $|\rho\rangle$ of the $[M]$:

$$
[M]|\rho\rangle = E(\rho)|\rho\rangle,\ \rho = 1, ..., f(\omega;\alpha) \qquad (4.5)
$$

These orthogonal eigenvectors are normalized by dividing by the square root of the corresponding eigenvalues. Coefficients of the normalized eigenvectors of e^{α}_{11} are

$$
\langle \omega j|\rho\alpha 1\rangle = \sum_{u=1}^{f(\omega;\alpha)} [e^{\alpha}_{11}]^{\omega}_{ju} \langle u|\rho\rangle / \sqrt{E(\rho)} \qquad (4.6)
$$

and from (3.12) the coefficients of the remaining elements of the symmetry-adapted basis are

$$
\langle \omega j|\rho\alpha r\rangle = \sum_{u=1}^{f(\omega;\alpha)} [e^{\alpha}_{r1}]^{\omega}_{ju} \langle u|\rho\rangle / \sqrt{E(\rho)} \qquad (4.7)
$$

V. ILLUSTRATION

The method described here is illustrated by the symmetry-adaptation of the 60 dimensional π-orbital basis for the Hückel treatment of icosahedral C_{60} fullerene. The characters, irreducible representations, and generators of the 120-order icosahedral point group $\mathscr{I}_h$ are given elsewhere as are the permutational representations of the generators over $B(\pi)$.[12,13] The five-dimensional irreducible representation H_g occurs three times so that the trace of $[e^{H_g}_{11}]^{\pi}$ is three. From eq 3.13, this matrix is computed by

$$
[e^{H_g}_{11}]^{\pi} = \frac{5}{120} \sum_{a=1}^{120} [G_a^{-1}]^{H_g}_{11} [G_a]^{\pi} \qquad (5.1)
$$

where the $[G_a]^{\pi}$ are permutation matrices composed of zeroes and ones. The first eight rows and columns of this 60×60 matrix, multiplied by 120 for convenient display, are given in Table 1.

Table 1. First Eight Rows and Columns of the 60×60 Matrix $[e^{H_g}_{11}]^{\pi}$, the Representation of the Projector $e^{H_g}_{11}$ for the Irreducible Representation H_g of the Icosahedral Point Group, $\mathscr{I}_h$, over the π Orbitals of Icosahedral Fullerene C_{60}[a]

$$
\begin{bmatrix}
10.0000 & 5.47746 & 8.27254 & 8.27254 & 5.47746 & -3.28648 & -6.00000 & -3.28648 \\
5.47746 & 9.13627 & 6.87500 & 6.87500 & 9.13627 & 4.33587 & -3.28648 & 4.33587 \\
8.27254 & 6.87500 & 7.73873 & 7.73873 & 6.87500 & -0.375000 & -4.96353 & -0.375000 \\
8.27254 & 6.87500 & 7.73873 & 7.73873 & 6.87500 & -0.375000 & -4.96353 & -0.375000 \\
5.47746 & 9.13627 & 6.87500 & 6.87500 & 9.13627 & 4.33587 & -3.28648 & 4.33587 \\
-3.28648 & 4.33587 & -0.375000 & -0.375000 & 4.33587 & 9.13627 & 5.47746 & 9.13627 \\
-6.00000 & -3.28648 & -4.96353 & -4.96353 & -3.28648 & 5.47746 & 10.0000 & 5.47746 \\
-3.28648 & 4.33587 & -0.375000 & -0.375000 & 4.33587 & 9.13627 & 5.47746 & 9.13627
\end{bmatrix}
$$

[a] The elements have been multiplied by 120, the order of the group, to give convenient numbers.

This matrix exhibits patterns typical of projection operator representations. First, it is symmetrical as required by the self-adjoint property. Second, a number of rows and columns are doubled and may be repeated even more frequently. Perhaps atypical in this case is the absence of off-diagonal zero values so that no column is orthogonal to another.

Direct projection would use the first three columns for the required projections. The value of the determinant of the upper left three by three block is effectively zero, however, indicating that this set is linearly dependent.

The systematic approach described here searches for the first nonzero column, number one in this example, then

Table 2. Eigenvalues and Corresponding Eigenvectors of the [*M*] Matrix from Eq 5.4[a]

	0.622102	12.5045	15.1460
1	0.557776	−0.487356	0.671841
2	−0.632515	0.274523	0.724267
6	0.537412	0.828928	0.155138

[a] Numbers in the left column denote columns of $[e_{11}^{H_g}]^{\pi}$. Each eigenvalue must be divided by 120 to give the correct unscaled value.

appends the next nonzero column, number two here. The appropriate [*M*] to six significant figures for these two vectors is

$$[M] = \begin{bmatrix} 10.0000 & 5.47746 \\ 5.47746 & 9.13627 \end{bmatrix} \tag{5.2}$$

having determinant of 61.3601, which is 4.26112×10^{-3} for the original quantities after division by the scaling factor $(120)^2$. Adding the third vector gives the [*M*] matrix

$$[M] = \begin{bmatrix} 10.0000 & 5.47746 & 8.27254 \\ 5.47746 & 9.13627 & 6.87500 \\ 8.27254 & 6.87500 & 7.73873 \end{bmatrix} \tag{5.3}$$

with determinant 6.36673×10^{-5} which is 3.68445×10^{-11} after division by $(120)^3$. This is certainly too small—effectively 0−10 places—so it is necessary to pick another column for the third choice. Since column four is identical to the third column and column five is identical to the second column, the next column that might work is the sixth, giving the [*M*] matrix

$$[M] = \begin{bmatrix} 10.0000 & 5.47746 & -3.28648 \\ 5.47746 & 9.13627 & 4.33587 \\ -3.28648 & 4.33587 & 9.13627 \end{bmatrix} \tag{5.4}$$

for which the determinant is 117.821 which is 6.81835×10^{-5} after division by $(120)^3$ and may be sufficiently large. The eigenvalues and eigenvectors of this matrix are given in Table 2 where each eigenvalue is to be divided by 120.

Other choices may give better conditioned [*M*] matrices. Taking the third choice to be column number seven gives

$$[M] = \begin{bmatrix} 10.0000 & 5.47746 & -6.00000 \\ 5.47746 & 9.13627 & -3.28648 \\ -6.00000 & -3.28648 & 10.0000 \end{bmatrix} \tag{5.5}$$

with determinant 392.705 which is 2.27260×10^{-4} after division by $(120)^3$. Eigenvalues and eigenvectors of this matrix are given in Table 3 where each eigenvalue is to be divided by 120.

Although both of these sets are linearly independent, the latter is computationally superior. A routine to find the set with largest determinant for the [*M*] matrix is feasible and may be desirable as dimensions and frequencies increase.

Table 3. Eigenvalues and Corresponding Eigenvectors of the Scaled [*M*] Matrix from Eq 5.5[a]

	3.18696	6.25758	19.6917
1	0.765939	0.0258983	0.642392
2	−0.453383	0.730191	0.511141
7	0.455831	0.682752	−0.571023

[a] Numbers in the left column denote columns of $[e_{11}^{H_g}]^{\pi}$. Each eigenvalue must be divided by 120 to give the correct unscaled value.

Table 4. H_g Symmetry-Adaptation Coefficients for Icosahedral C_{60} Hückel Basis Corresponding to the Scaled [*M*] in Eq 5.5 and the Eigenvectors in Table 3, Normalized According to (4.6)[a]

$$\langle \pi i|\pi;1H_g1\rangle = [e_{11}^{H_g}]_{i1}^{\pi} \times 4.69999 + [e_{11}^{H_g}]_{i2}^{\pi} \times (-2.78207) + [e_{11}^{H_g}]_{i7}^{\pi} \times 2.79709$$

$$\langle \pi i|\pi;2H_g1\rangle = [e_{11}^{H_g}]_{i1}^{\pi} \times 0.113411 + [e_{11}^{H_g}]_{i2}^{\pi} \times 3.19759 + [e_{11}^{H_g}]_{i7}^{\pi} \times 2.98985$$

$$\langle \pi i|\pi;3H_g1\rangle = [e_{11}^{H_g}]_{i1}^{\pi} \times 1.58580 + [e_{11}^{H_g}]_{i2}^{\pi} \times 1.26180 + [e_{11}^{H_g}]_{i7}^{\pi} \times (-1.40962)$$

[a] Each eigenvalue in Table 3 was divided by 120 before normalization.

The symmetry-adaptation coefficients obtained by eq 4.6 from this last choice are displayed in Table 4.

VI. CONCLUSION

The method described here will systematically symmetry-adapt a basis of any finite size. If the inner product matrix, [*M*], can be diagonalized, the transformation can be made unitary, and the result is a unitary transformation from the defining basis to a suitably conditioned symmetry-adapted basis that will be orthonormal if the defining basis is orthonormal. If the absolute value of the determinant of [*M*] is sufficiently large, the corresponding $f(\omega;\alpha)$ columns of $[e_{11}^{\alpha}]^{\omega}$ are linearly independent and can be used as nonorthogonal elements of a symmetry-adapted basis.

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