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On the Symmetry Point Groups for Some Simple Parameter-Dependent Symmetric Matrices

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Abstract: We try to determine the groups of orthogonal matrices that commute with a given simple parameter-dependent symmetric matrix. To this end we resort to a graphical representation of the latter that enables us to find the group of matrices from the symmetry elements of the figure. This strategy works fine for all values of the model parameter λ except for $\lambda = -1$. In order to obtain the symmetry point group in this particular case we have to resort to alternative procedures.

Keywords: group theory; symmetric matrix; degeneracy; character table

1. Introduction

Point group symmetry is a most useful tool for the analysis of many properties of polyatomic molecules [1,2]. It is relevant in the discussion of several features of spectroscopy as well as in the application of quantum mechanics to the electronic structure of polyatomic molecules in their equilibrium geometry. The determination of a suitable point group for a given molecule is based on the identification of the symmetry elements on the graphical representation of the molecule.

In this paper we discuss some Hückel-like symmetric matrices [2] that depend on a parameter and can be represented graphically. The identification of the symmetry elements for some values of the parameter follows the rules commonly used in the analysis of molecules [1,2] but for a particular value of the parameter the graphical representation is misleading. The identification of the point group symmetry for this particular value of the matrix parameter requires an alternative procedure.

In the short section 2 we outline the main idea of the paper. In sections 3 and 4 we discuss examples of three- and fourth- dimensional parameter-dependent symmetric matrices and derive the orthogonal matrices that commute with them. In particular, we determine the symmetry point groups for all values of the model parameter. Finally, in section 5 we summarize the main results of the paper and draw conclusions.

2. Point Group for a Symmetric Matrix

The purpose of this paper is to find out the group of orthogonal matrices $\mathbf{U}_i$, $i = 1, 2, \ldots, M$ that commute with a given symmetric matrix $\mathbf{H}(\lambda)$ of dimension N that depends on a parameter λ. The symmetric matrix can be represented by a figure with vertices v_i, $i = 1, 2, \ldots, N$ (for example, a polygon). Instead of the matrices $\mathbf{U}_i$ we will show their effect on a vector of vertices v_i as $(v_1, v_2, \ldots, v_N) \to (v_1, v_2, \ldots, v_N) \cdot \mathbf{U}_i$. In order to identify the corresponding point group we obtain the classes and orders of all the group elements $\mathbf{U}_i$ [1,2]. In what follows we consider two illustrative examples.

3. Three-Dimensional Matrix

The first example is given by the symmetric matrix

$$\mathbf{H}(\lambda) = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & \lambda \\ 1 & \lambda & 0 \end{pmatrix}. \tag{1}$$

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In order to obtain the orthogonal matrices that commute with it, we resort to the graphical representation of $\mathbf{H}(\lambda)$ shown in Figure 1. When $\lambda \neq 1$ the symmetry operations for the isosceles triangle are

$$(v_1, v_2, v_3) \rightarrow \begin{cases} (v_1, v_2, v_3) \\ (v_1, v_3, v_2) \end{cases}, \tag{2}$$

that leads to a group of two matrices that is isomorphic with the point group C_2 [1,2]. Since $\mathbf{H}(\lambda)$ also commutes with $-\mathbf{U}_i$, then we can build a larger group of four matrices that is isomorphic with the point group C_{2v} [1,2]. Neither C_2 or C_{2v} predict degeneracy.

When $\lambda = 1$ the triangle in Figure 1 is equilateral and there is a three-fold rotation axis through the center of the figure that leads to the symmetry operations

$$(v_1, v_2, v_3) \rightarrow \begin{cases} (v_1, v_2, v_3) \\ (v_3, v_1, v_2) \\ (v_2, v_3, v_1) \end{cases}, \tag{3}$$

that is a matrix representation of the point group C_3. If we add the reflection planes perpendicular to the triangle we have

$$(v_1, v_2, v_3) \rightarrow \begin{cases} (v_1, v_2, v_3) \\ (v_3, v_1, v_2) \\ (v_2, v_3, v_1) \\ (v_1, v_3, v_2) \\ (v_2, v_1, v_3) \\ (v_3, v_2, v_1) \end{cases}, \tag{4}$$

that is a matrix representation of C_{3v} [1,2]. If we add the matrices $-\mathbf{U}_i$ we obtain a matrix representation of the point group D_{3h} [1,2]. Both C_{3v} and D_{3h} predict two-fold degeneracy.

The eigenvalues of the matrix $\mathbf{H}(\lambda)$

$$E_1 = -\lambda,\ E_2 = \frac{\lambda - \sqrt{\lambda^2 + 8}}{2},\ E_3 = \frac{\sqrt{\lambda^2 + 8} + \lambda}{2}, \tag{5}$$

are shown in Figure 2. We appreciate that there is no degeneracy when $\lambda \neq 1$ and that two eigenvalues coalesce at $\lambda = 1$ in agreement with the point groups C_{2v} and C_{3v}, respectively, derived above. An exception is the case $\lambda = -1$ that exhibits a two-fold degeneracy that may be considered accidental because it cannot be explained by the graphical argument used above. However, this degeneracy is not accidental.

In order to obtain the group of orthogonal matrices that commute with $\mathbf{H}(-1)$ we resort to a sort of brute-force procedure. We choose an arbitrary matrix $\mathbf{U}$ and try to solve the equations$[\mathbf{H}(-1), \mathbf{U}] = \mathbf{0}$ (the zero matrix) and $\mathbf{U}^t\mathbf{U} = \mathbf{I}$ (the identity matrix), where $[,]$ denotes a commutator t stands for transpose. We only need a matrix different from those shown in equation (2) because we can obtain the remaining ones by products of pairs of matrices. In this way we derived a group of matrices that yield the transformations

$$(v_1, v_2, v_3) \rightarrow \begin{cases} (v_1, v_2, v_3) \\ (v_1, v_3, v_2) \\ (-v_3, v_2, -v_1) \\ (-v_3, -v_1, v_2) \\ (-v_2, v_3, -v_1) \\ (-v_2, -v_1, v_3) \end{cases}, \tag{6}$$

that is a matrix representation of the group C_{3v}. If we add the matrices $-\mathbf{U}_i$ we obtain a matrix representation of the group D_{3h}. Both groups predict two-fold degeneracy in agreement with Figure 2.

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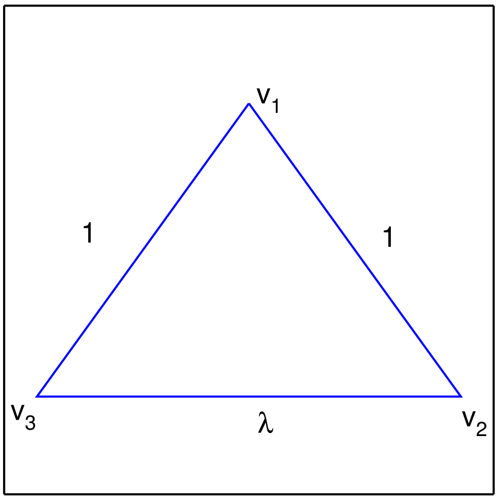

Figure 1. Graphical representation of the matrix (1).

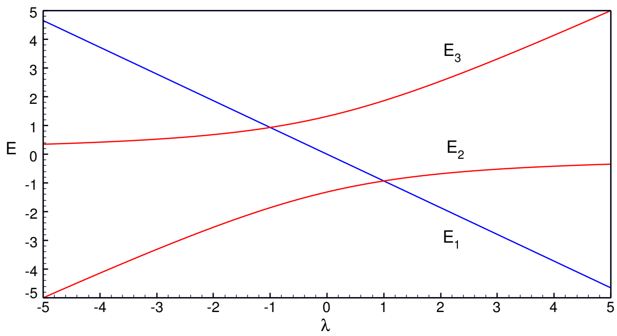

Figure 2. Eigenvalues of the matrix (1).

4. Fourth-Dimensional Matrix

The second example is given by the matrix

$$\mathbf{H}(\lambda) = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \lambda \\ 1 & 0 & \lambda & 0 \end{pmatrix}, \tag{7}$$

that is represented in Figure 3. When $\lambda \neq 1$ (rectangle) we expect the symmetry operations

$$(v_1, v_2, v_3, v_4) \rightarrow \begin{cases} (v_1, v_2, v_3, v_4) \\ (v_2, v_1, v_4, v_3) \end{cases}, \tag{8}$$

which are a representation of the point group C_2. If we add the matrices $-\mathbf{U}_i$ we have the point group C_{2v}.

The most symmetric object appears when $\lambda = 1$ (square) that exhibits a four-fold rotation axis perpendicular to the figure and the related operations

$$(v_1, v_2, v_3, v_4) \rightarrow \begin{cases} (v_1, v_2, v_3, v_4) \\ (v_4, v_1, v_2, v_3) \\ (v_3, v_4, v_1, v_2) \\ (v_2, v_3, v_4, v_1) \end{cases}, \tag{9}$$

lead to a matrix representation of the group C_4 [1,2]. If we add the matrices $-\mathbf{U}_i$ we obtain the group C_{4h} [1,2].

If we consider all the reflection planes perpendicular to the plane of the figure we have

$$(v_1, v_2, v_3, v_4) \rightarrow \begin{cases} (v_1, v_2, v_3, v_4) \\ (v_4, v_1, v_2, v_3) \\ (v_3, v_4, v_1, v_2) \\ (v_2, v_3, v_4, v_1) \\ (v_1, v_4, v_3, v_2) \\ (v_2, v_1, v_4, v_3) \\ (v_3, v_2, v_1, v_4) \\ (v_4, v_3, v_2, v_1) \end{cases}, \tag{10}$$

that is a matrix representation of the point group C_{4v} [1,2]. If we add the matrices $-\mathbf{U}_i$ we obtain a representation of the point group D_{4h} [1,2]. The conclusion is that there should be no degeneracy when $\lambda \neq 1$ and two-fold degeneracy when $\lambda = 1$.

The eigenvalues of the matrix (7)

$$\begin{aligned} E_1 &= \frac{1+\lambda}{2} - \frac{\sqrt{\lambda^2 - 2\lambda + 5}}{2},\; E_2 = -\frac{1+\lambda}{2} - \frac{\sqrt{\lambda^2 - 2\lambda + 5}}{2}, \\ E_3 &= \frac{1+\lambda}{2} + \frac{\sqrt{\lambda^2 - 2\lambda + 5}}{2},\; E_4 = -\frac{1+\lambda}{2} + \frac{\sqrt{\lambda^2 - 2\lambda + 5}}{2}, \end{aligned} \tag{11}$$

are shown in Figure 4. The groups derived above account for the non-degeneracy when $\lambda \neq 1$ and the two-fold degeneracy at $\lambda = 1$. However, as in the preceding example our analysis fails for $\lambda = -1$ where we find two sets of two-fold degenerate eigenvalues.

In order to obtain the matrices that commute with $\mathbf{H}(-1)$ we followed the brute-force procedure outlined in the preceding section and obtained

$$(v_1, v_2, v_3, v_4) \rightarrow \begin{cases} (v_1, v_2, v_3, v_4) \\ (v_2, v_3, -v_4, v_1) \\ (v_3, -v_4, -v_1, v_2) \\ (v_4, v_1, v_2, -v_3) \\ (-v_4, -v_1, -v_2, v_3) \\ (-v_3, v_4, v_1, -v_2) \\ (-v_2, -v_3, v_4, -v_1) \\ (-v_1, -v_2, -v_3, -v_4) \end{cases} \tag{12}$$

that is a matrix representation of the point group C_8 [1,2].

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In order to obtain a larger group we added the two matrices in equation (8) and carried out all the products thus ending with a set of 16 matrices that produce the following transformations

$$
(v_1, v_2, v_3, v_4) \to \begin{cases}
(v_1, v_2, v_3, v_4) \\
(v_2, v_1, v_4, v_3) \\
(v_1, v_4, -v_3, v_2) \\
(v_2, v_3, -v_4, v_1) \\
(v_4, v_1, v_2, -v_3) \\
(v_3, v_2, v_1, -v_4) \\
(v_3, -v_4, -v_1, v_2) \\
(v_4, -v_3, -v_2, v_1) \\
(-v_4, v_3, v_2, -v_1) \\
(-v_3, v_4, v_1, -v_2) \\
(-v_3, -v_2, -v_1, v_4) \\
(-v_1, -v_4, v_3, -v_2) \\
(-v_4, -v_1, -v_2, v_3) \\
(-v_2, -v_3, v_4, -v_1) \\
(-v_2, -v_1, -v_4, -v_3) \\
(-v_1, -v_2, -v_3, -v_4)
\end{cases}, \tag{13}
$$

and that are a representation of the point group D_8(http://symmetry.jacobs-university.de/). Both C_8 and D_8 account for the two-fold degeneracy at $\lambda = -1$.

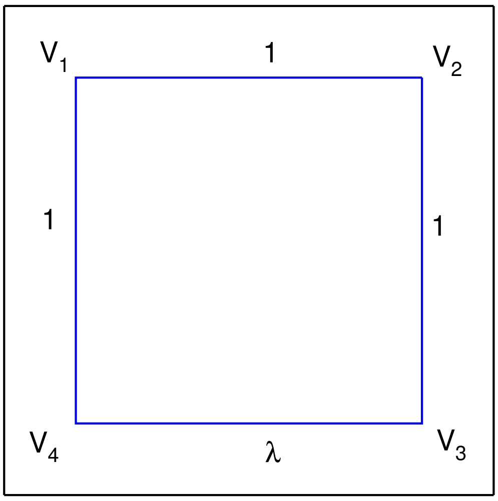

Figure 3. Graphical representation of the matrix (7).

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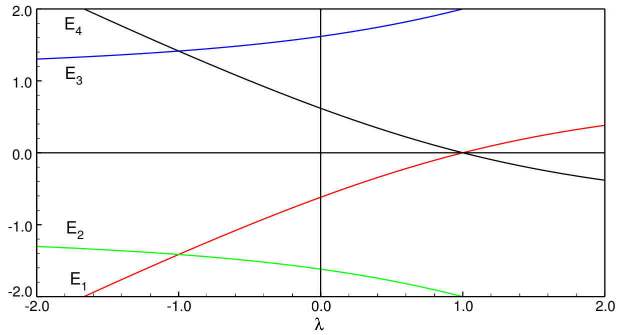

Figure 4. Eigenvalues of the matrix (7).

5. Conclusions

It is clear that the graphical representation of the matrix is useful for the identification of the symmetry point group for all the values of the model parameter except for $\lambda = -1$ that requires a particular treatment. It is not clear to us the reason for this baffling behaviour of the simple Hückel-like matrices.

References

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