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Symmetric Graphs – Spectra and Eigenvectors

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Abstract

Davidson (1981) developed a general procedure, based on group representation theory, for determining the spectra of graphs distinguished by a certain rotational symmetry, with application to molecular graphs. In this paper a more general method, applicable to any arbitrarily arc weighted directed graph that has a non-trivial automorphism, and yielding both eigenvalues and eigenvectors, is developed. The proofs, elementary and straightforward, avoid the use of the theory of group characters altogether.

Key words: arc weighted graph, permutation, automorphism, symmetry group, eigenvectors, eigenvalues, spectrum, applications to chemistry (LCAO-MO theory)

1 Introduction

In 1981 R.A. Davidson [2] published a reduction procedure, based on group representation theory, which allows the spectrum of a finite weighted graph endowed with a certain rotational symmetry to be calculated from spectra of smaller graphs, a method with rich applications in the theory of molecular graphs, in particular, of hydrocarbons and related compounds [3]. Here we shall develop an extended method, applicable to any finite directed (undirected) graph G with arbitrary complex arc (edge) weights that has a non-trivial automorphism, yielding the spectrum via the eigenvectors of G.

A remarkable feature is the fact that all proofs are quite elementary and straightforward: stressing this aspect we shall avoid any reference to group representation theory (group characters).

2 Definitions, Notation, Terminology

Let $\mathbb{G} = (V, A)$ be a finite directed graph (multiple arcs and loops being admitted) on n vertices whose arcs are arbitrarily weighted with complex numbers – briefly called a *graph*.

An arc from vertex x to vertex y with weight w is denoted $a = a[w] = [x, y; w]$ (Fig. 2.1). Every non-arc is considered a "zero arc", i.e., an arc a with weight zero: $a[0] = [x, y; 0]$.

A multiple (k-fold) arc – i.e., a set of parallel arcs $a_i = [x, y; w_i], i = 1, 2, \ldots, k$ – may be replaced with a single arc a whose weight is the sum of the w_i: $a = [x, y; \sum_{i=1}^{k} w_i]$.

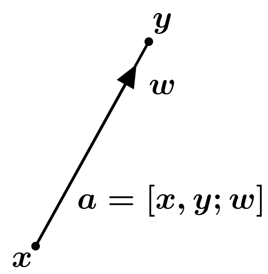


Figure 2.1: Arc a from x to y with weight w

An undirected edge $(x, y; w)$ is equivalent to, and replaced by, the pair of antiparallel arcs $[x, y; w]$, $[y, x; w]$.

It is convenient to assume that, for every ordered pair $[x, y]$ of vertices, there is in $\mathbb{G}$ precisely one arc a from x to y: $a = [x, y; w]$ where $x = y$ and $w = 0$ are allowed. Therefore, whenever a multiple arc $\{[x, y; w_i] \mid i = 1, 2, \ldots, k\}$ is encountered, it will be considered a single arc $[x, y; \sum_{i=1}^{k} w_i]$. Thus the ordered pair $[x, y]$ uniquely determines an arc $a = a(x, y) = [x, y; w]$ with weight $w = w(a) = w(x, y)$.

Let, for the moment, $V = \{1, 2, \ldots, n\}$ and define the *weight matrix* (weighted adjacency matrix) W of $\mathbb{G}$ by $\mathsf{W} = (w(i, j))_{i,j=1,2,\ldots,n}$.[a]

The symmetry group of $\mathbb{G}$, consisting of all automorphisms of $\mathbb{G}$, is isomorphic to the group of permutations P of the vertex set of $\mathbb{G}$ that leave the weight function w invariant, or, equivalently, of all permutation matrices P satisfying $\mathsf{P}^{-1}\mathsf{W}\mathsf{P} = \mathsf{W}$; we shall identify an automorphism with the permutation P that describes it. Graph $\mathbb{G}$ is called *symmetric* iff[b] its symmetry group is non-trivial.

Let P be an arbitrary non-trivial automorphism of $\mathbb{G}$ consisting of disjoint cycles $C_1, C_2, \ldots, C_r$ (including cycles of length one) where cycle C_ϱ has length s_ϱ and contains vertices $x_{\varrho\sigma}$, $\sigma = 0, 1, \ldots, s_\varrho - 1$:

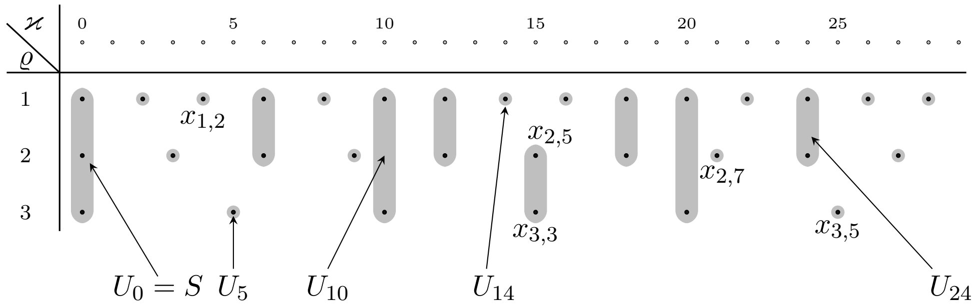
$$P = C_1 C_2 \cdots C_r, \quad C_\varrho = (x_{\varrho 0}\, x_{\varrho 1} \cdots x_{\varrho, s_\varrho - 1}).$$

Set $\tilde{C}_\varrho = \{x_{\varrho\sigma} \mid \sigma = 0, 1, \ldots, s_\varrho - 1\}$.

Let M denote the least common multiple of the cycle lengths s_ϱ of P and arrange the vertices according to the following (cyclic) cartesian scheme $\mathcal{H} = \mathcal{H}(P)$: the rows are R_ϱ ($\varrho = 1, 2, \ldots, r$), the columns are $S_\varkappa$ ($\varkappa = 0, 1, \ldots, M - 1$) which may be cyclically repeated by $S_M = S_0$, $S_{M+1} = S_1$, etc. . Row R_ϱ contains the cycle C_ϱ, the vertices in R_ϱ are arranged in equidistant positions, i.e., $x_{\varrho\sigma}$ is placed in row R_ϱ and in column $S_{\varkappa(\varrho,\sigma)}$ where $\varkappa(\varrho, \sigma) = \dfrac{M}{s_\varrho}\sigma$ ($\varrho = 1, 2, \ldots, r; \quad \sigma = 0, 1, \ldots, s_\varrho - 1$) (Fig. 2.2).

[a]Note the one-to-one correspondence between the set of graphs (as defined above) with labelled vertices and the set of square matrices with complex entries.

[b]We use *iff* for *if and only if* if and only if "if and only if" (briefly,"iff") is part of a definition.



P and $\mathcal{H}(P)$.

The parameters of P are: $r = 3$; $s_1 = 15$, $s_2 = 10$, $s_3 = 6$; $M = 30$.

The shaded areas contain the subsets $U_\varkappa$ of $V(\mathbb{G})$, e.g., $U_4 = \{x_{1,2}\}$, $U_{15} = \{x_{2,5}, x_{3,3}\}$.

Figure 2.2: An example of $\mathcal{H}(P)$

Column $S_\varkappa$ contains the set

$$U_\varkappa = \{x_{\varrho\sigma} \mid \frac{M}{s_\varrho}\sigma = \varkappa\}$$

which may be empty. Let $K = \{\varkappa \mid U_\varkappa \neq \varnothing\}$. Vertex set $V(\mathbb{G})$ decomposes into (disjoint non-empty) sets $U_\varkappa$:

$$V(\mathbb{G}) = \dot{\bigcup}_{\varkappa \in K} U_\varkappa \qquad \text{(Fig. 2.2).}$$

We shall abbreviate S_0, $x_{\varrho\sigma}$ and $x_{\varrho 0}$ by S, $\varrho\sigma$ and $\varrho\,(=\varrho 0)$, respectively. Thus

$$S = S_0 = \{1, 2, \ldots, r\}.$$

Let $d(\alpha, \beta)$ and $m(\alpha, \beta)$ denote the greatest common divisor and the least common multiple of s_α, s_β and define

$$g(\alpha, \beta) = s_\beta / d(\alpha, \beta) = m(\alpha, \beta)/s_\alpha. \tag{2.1}$$

3 Consequences of the symmetry

By cyclicity the weight function $w(\varrho_1\sigma_1, \varrho_2\sigma_2)$ can be defined for all integers σ_1, σ_2. So extended, $w(\varrho_1\sigma_1, \varrho_2\sigma_2)$ (ϱ_1, ϱ_2 fixed) is periodic in σ_1 with period s_{ϱ_1} and in σ_2 with period s_{ϱ_2}. Whenever necessary, a σ argument is reduced modulo its respective period. The above implies that whenever for some integers q_1, q_2 the equation

$$\sigma_1' - \sigma_1 + q_1 s_{\varrho_1} = \sigma_2' - \sigma_2 + q_2 s_{\varrho_2}$$

holds then

$$w(\varrho_1\sigma_1', \varrho_2\sigma_2') = w(\varrho_1\sigma_1, \varrho_2\sigma_2).$$

The set of numbers $q_1 s_{\varrho_1} - q_2 s_{\varrho_2}$ being identical with the set of multiples of $d(\varrho_1, \varrho_2)$ we conclude:

(A) $\sigma_1' - \sigma_2' \equiv \sigma_1 - \sigma_2, \mod d(\varrho_1, \varrho_2)$
implies $w(\varrho_1\sigma_1', \varrho_2\sigma_2') = w(\varrho_1\sigma_1, \varrho_2\sigma_2)$.

4 The reduction procedure

For every $\varkappa \in K$ we shall construct a graph $\mathbb{G}(\varkappa) = (V_\varkappa, A_\varkappa)$ on $|U_\varkappa|$ vertices. $V_\varkappa$, the vertex set of $\mathbb{G}(\varkappa)$, is the projection of $U_\varkappa$ into S:

$$V_\varkappa = \{\varrho \mid \varrho\sigma \in U_\varkappa\}.$$

To define the arc set $A_\varkappa$ let $\varepsilon = \exp(2\pi i/M)$ and

$$\tilde{U}_\varkappa = \bigcup_{\varrho \in V_\varkappa} \tilde{C}_\varrho = \{\varrho\sigma \mid \varrho \in V_\varkappa, \quad \sigma = 0, 1, \ldots, s_\varrho - 1\}.$$

Every arc $z = [x_1, x_2; w]$ of $\mathbb{G}$ with $x_1 = \varrho_1 \in V_\varkappa$, $x_2 = \varrho_2\sigma \in \tilde{U}_\varkappa$ is in $\mathbb{G}(\varkappa)$ replaced by the arc $\hat{z}' = [x_1', x_2'; \hat{w}_\varkappa']$ with $x_1' = x_1 = \varrho_1 \in V_\varkappa$, $x_2' = \varrho_2 \in V_\varkappa$, $\hat{w}_\varkappa' = w \cdot \varepsilon^{\varkappa\sigma}$. Note that all arcs with both their ends in $V_\varkappa$ are retained in $\mathbb{G}(\varkappa)$. The arcs $\hat{z}'$ with fixed ends $x_1' = \varrho_1$, $x_2' = \varrho_2$ ($\varrho_1, \varrho_2 \in V_\varkappa$) are united to form in $\mathbb{G}(\varkappa)$ the single arc $z' = [\varrho_1, \varrho_2; w_\varkappa']$ where

(B) $$w_\varkappa' = w_\varkappa'(\varrho_1, \varrho_2) = \sum \hat{w}_\varkappa' = \sum_{\sigma=0}^{s_{\varrho_1}-1} w(\varrho_1, \varrho_2\sigma)\varepsilon^{\varkappa\sigma}.$$

The resulting set of arcs is $A_\varkappa$.
Note that $\mathbb{G}(0)$ is a front divisor of $\mathbb{G}$ (see [1], Chapter 4 and Section 5.3).

5 Claims

Let, for fixed $\varkappa \in K$, $\mathbf{u} = \{u(\varrho) \mid \varrho \in V_\varkappa\}$ be an eigenvector of $\mathbb{G}(\varkappa)$ with corresponding eigenvalue λ, i. e., assume that

(C) $\mathbf{u} \neq \mathbf{0}$ *and* λ *satisfy the equation*
$\sum_{\varrho \in V_\varkappa} w_\varkappa'(\varrho_0, \varrho)u(\varrho) = \lambda u(\varrho_0)$ $(\varrho_0 \in V_\varkappa)$.

The *extended eigenvector* $\mathbf{u}'$ is defined on S by

$$u'(\varrho) = \begin{cases} u(\varrho) & \text{if } \varrho \in V_\varkappa, \\ 0 & \text{if } \varrho \in S - V_\varkappa. \end{cases}$$

Let

(D) $\mathbf{v} = \{v(\varrho\sigma) \mid \varrho\sigma \in V(\mathbb{G})\}$
where $v(\varrho\sigma) = \begin{cases} u(\varrho) \cdot \varepsilon^{\varkappa\sigma} & \textit{if } \varrho\sigma \in \tilde{U}_\varkappa \ (\textit{i.e., if } \varrho \in V_\varkappa) \\ 0 & \textit{otherwise} \ (\textit{i.e., if } \varrho \in S - V_\varkappa). \end{cases}$

Theorem 5.1. $\mathbf{v}$ *and* λ *are an eigenvector and corresponding eigenvalue of* $\mathbb{G}$ *, i.e.,* $\mathbf{v}$ *and* λ *satisfy the equation*

$$\sum_{\varrho\sigma\in V(\mathbb{G})} w(\varrho_0\sigma_0,\varrho\sigma)v(\varrho\sigma) = \lambda v(\varrho_0\sigma_0) \qquad (\varrho_0\sigma_0 \in V(\mathbb{G})).$$

Theorem 5.2. *Eigenvectors* $\mathbf{v}$ *of* $\mathbb{G}$ *obtained from linearly independent extended eigenvectors* $\mathbf{u}'$ *of the* $\mathbb{G}(\varkappa)$ *are linearly independent.*

Theorem 5.3. *Let* $\varkappa_1 \neq \varkappa_2$*. Eigenvectors* $\mathbf{v}_1$*,* $\mathbf{v}_2$ *of* $\mathbb{G}$ *obtained from eigenvectors* $\mathbf{u}_1$ *of* $\mathbb{G}(\varkappa_1)$ *and* $\mathbf{u}_2$ *of* $\mathbb{G}(\varkappa_2)$ *are orthogonal.*

6 Proofs

Proof of Theorem 5.1

Let $\varkappa \in K$ (fixed), $\varrho_0\sigma_0 \in V(\mathbb{G})$, set $\varepsilon^{\varkappa} = \omega$ and abbreviate

$$\sum_{\varrho\sigma\in V(\mathbb{G})} w(\varrho_0\sigma_0,\varrho\sigma)v(\varrho\sigma) = Q. \tag{6.1}$$

We have to show: $Q = \lambda v(\varrho_0\sigma_0)$.

Because of **(D)** (Section 5) (6.1) reduces to

$$Q = \sum_{\varrho\in V_\varkappa}\sum_{\sigma=0}^{s_\varrho-1} w(\varrho_0\sigma_0,\varrho\sigma)u(\varrho)\omega^{\sigma}.$$

Recall: $\varkappa = \dfrac{M}{s_\varrho}\sigma^*$ for some $\sigma^* < s_\varrho$, thus

$$\omega = \exp\left(\frac{2\pi i}{M}\varkappa\right) = \exp\left(\frac{2\pi i}{s_\varrho}\sigma^*\right)$$

is an s_ϱ-th root of unity. Therefore, both $w(\varrho_0\sigma_0,\varrho\sigma)$ and ω^σ are periodic in σ with period s_ϱ for every $\varrho \in V_\varkappa$. This implies

$$\begin{aligned} Q &= \sum_{\varrho\in V_\varkappa}\sum_{\sigma=0}^{s_\varrho-1} w(\varrho_0\sigma_0,\varrho(\sigma+\sigma_0))u(\varrho)\omega^{\sigma+\sigma_0} \\ &= \omega^{\sigma_0}\sum_{\varrho\in V_\varkappa} u(\varrho)\sum_{\sigma=0}^{s_\varrho-1} w(\varrho_0\sigma_0,\varrho(\sigma+\sigma_0))\omega^{\sigma}. \end{aligned}$$

By **(A)** (Section 3), $w(\varrho_0\sigma_0,\varrho(\sigma+\sigma_0)) = w(\varrho_0,\varrho\sigma)$, therefore,

$$Q = \omega^{\sigma_0}\sum_{\varrho\in V_\varkappa} u(\varrho)\sum_{\sigma=0}^{s_\varrho-1} w(\varrho_0,\varrho\sigma)\omega^{\sigma}. \tag{6.2}$$

We distinguish two cases. **Case 1:** $\varrho_0 \in V_\varkappa$; **Case 2:** $\varrho_0 \notin V_\varkappa$.

Case 1. Because of **(B)** (Section 4),

$$Q = \omega^{\sigma_0} \sum_{\varrho \in V_\varkappa} w'_\varkappa(\varrho_0, \varrho) u(\varrho)$$

which, by **(C)** and **(D)** (Section 5), implies

$$Q = \omega^{\sigma_0} \cdot \lambda u(\varrho_0) = \lambda v(\varrho_0 \sigma_0), \text{ as claimed.}$$

Case 2. To show: $Q = 0$.

Abbreviate $d(\varrho_0, \varrho) = d$, $m(\varrho_0, \varrho) = m$, $g(\varrho_0, \varrho) = g$.

First we show

(I) ω^d is a g^{th} root of unity,

(II) $\omega^d \neq 1$.

We have $\varkappa = \frac{M}{s_\varrho}\sigma^*$ where $\sigma^* < s_\varrho$; $d = \frac{s_\varrho}{g}$, thus $\varkappa d = \frac{M}{g}\sigma^*$ and

$$\omega^d = \exp\left(\frac{2\pi i}{M}\varkappa d\right) = \exp\left(\frac{2\pi i}{g}\sigma^*\right).$$

This proves (I).

To prove (II) we shall show that σ^*/g is not an integer.

Assume that $\sigma^*/g = \alpha$ is an integer. Let $\beta = m/s_\varrho$, $\tau = \alpha\beta$, both being integers. We have (see (2.1))

$$\tau = \frac{\sigma^*}{g} \cdot \frac{m}{s_\varrho} = \frac{\sigma^*}{s_\varrho} \cdot s_{\varrho_0}. \tag{6.3}$$

$\sigma^*/s_\varrho < 1$ implies $\tau < s_{\varrho_0}$. From (6.3) we conclude $\frac{M}{s_{\varrho_0}}\tau = \frac{M}{s_\varrho}\sigma^* = \varkappa$ which means that $\varrho_0\tau \in U_\varkappa$, thus $\varrho_0 \in V_\varkappa$; this contradiction proves (II).

As a consequence of (I) and (II),

$$\sum_{\gamma=0}^{g-1} \left(\omega^d\right)^\gamma = 0. \tag{6.4}$$

Now we resume (6.2) which we write as

$$Q = \omega^{\sigma_0} \sum_{\varrho \in V_\varkappa} u(\varrho) \cdot Q_\varrho, \quad Q_\varrho = \sum_{\sigma=0}^{s_\varrho - 1} w(\varrho_0, \varrho\sigma)\omega^\sigma.$$

We set $\sigma = \delta + \gamma d$; note that summation over σ ($\sigma = 0, 1, \ldots, s_\varrho - 1$) is the same as summation over δ, γ ($\delta = 0, 1, \ldots, d-1$; $\gamma = 0, 1, \ldots, g-1$).

We have

$$Q_\varrho = \sum_{\gamma=0}^{g-1} \sum_{\delta=0}^{d-1} w(\varrho_0, \varrho(\delta + \gamma d))\omega^{\delta + \gamma d}.$$

By **(A)** (Section 3), this reduces to

$$Q_\varrho = \sum_{\delta=0}^{d-1} \sum_{\gamma=0}^{g-1} w(\varrho_0, \varrho\delta)\omega^\delta \omega^{\gamma d} = \sum_{\delta=0}^{d-1} w(\varrho_0, \varrho\delta)\omega^\delta \sum_{\gamma=0}^{g-1} \left(\omega^d\right)^\gamma$$

which by (6.4) implies $Q_\varrho = 0$, thus $Q = 0$, as claimed.

Theorem 5.1 is now proved. □

Proof of Theorem 5.2

Assume that eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m$ of $\mathbb{G}$ that have been obtained from linearly independent extended eigenvectors $\mathbf{u}'_\mu$ of the $\mathbb{G}(\varkappa)$ are linearly dependent. Then there are numbers $c_1, c_2, \ldots, c_m$, not all equal to zero, such that $\sum_{\mu=1}^{m} c_\mu \mathbf{v}_\mu = \mathbf{0}$ or, equivalently,

$$\sum_{\mu=1}^{m} c_\mu v_\mu(\varrho\sigma) = 0, \quad \varrho = 1, 2, \ldots, r; \quad \sigma = 0, 1, \ldots, s_\varrho - 1.$$

True in particular for $\sigma = 0$ which by **(D)** (Section 5) implies

$$\sum_{\mu=1}^{m} c_\mu v_\mu(\varrho) = \sum_{\mu=1}^{m} c_\mu u'_\mu(\varrho) = 0, \quad \varrho = 1, 2, \ldots, r, \text{ thus } \sum_{\mu=1}^{m} c_\mu \mathbf{u}'_\mu = \mathbf{0},$$

contradicting the linear independence of the vectors $\mathbf{u}'_\mu$. □

Proof of Theorem 5.3

Assume $\varkappa_1 \neq \varkappa_2$ and let $\mathbf{v}_1$ and $\mathbf{v}_2$ be eigenvectors of graph $\mathbb{G}$ derived from eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$ of graphs $\mathbb{G}(\varkappa_1)$ and $\mathbb{G}(\varkappa_2)$, respectively. We shall show that $\mathbf{v}_1 \cdot \mathbf{v}_2$ (the scalar product of $\mathbf{v}_1$ and $\mathbf{v}_2$) equals zero. We have

$$\mathbf{v}_1 \cdot \mathbf{v}_2 = \sum_{\varrho=1}^{r} c_\varrho \text{ where } c_\varrho = \sum_{\sigma=0}^{s_\varrho - 1} v_1(\varrho\sigma)\overline{v_2(\varrho\sigma)}.$$

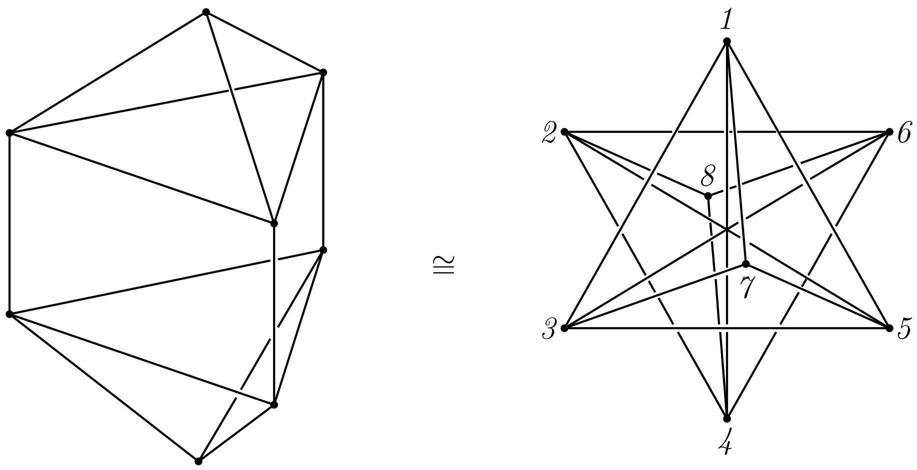
If $\varrho \notin V_{\varkappa_1} \cap V_{\varkappa_2}$ then, by **(D)**, at least one of $v_1(\varrho\sigma)$, $v_2(\varrho\sigma)$ is zero, thus $c_\varrho = 0$. Assume $\varrho \in V_{\varkappa_1} \cap V_{\varkappa_2}$. By **(D)**,

$$c_\varrho = \sum_{\sigma=0}^{s_\varrho - 1} u'_1(\varrho)\, \varepsilon^{\varkappa_1 \sigma}\, \overline{u'_2(\varrho)}\, \varepsilon^{-\varkappa_2 \sigma} = u'_1(\varrho)\overline{u'_2(\varrho)} \sum_{\sigma=0}^{s_\varrho - 1} \varepsilon^{(\varkappa_1 - \varkappa_2)\sigma}.$$

Recall: $\varepsilon = \exp(2\pi i/M)$, $\varkappa_i = \frac{M}{s_\varrho}\sigma_i^*$ where $0 \leq \sigma_i^* < s_\varrho$; note that $|\sigma_1^* - \sigma_2^*| < s_\varrho$ and, because of $\varkappa_1 \neq \varkappa_2$, also $\sigma_1^* \neq \sigma_2^*$, thus $0 < |\sigma_1^* - \sigma_2^*| < s_\varrho$. Therefore, $\varepsilon^{\varkappa_1 - \varkappa_2} = \exp(2\pi i(\sigma_1^* - \sigma_2^*)/s_\varrho)$ is an s_ϱ-th root of unity distinct from 1 implying

$$\sum_{\sigma=0}^{s_\varrho - 1} \varepsilon^{(\varkappa_1 - \varkappa_2)\sigma} = 0.$$

As immediate consequences, $c_\varrho = 0$ and $\mathbf{v}_1 \cdot \mathbf{v}_2 = \sum_{\varrho=1}^{r} c_\varrho = 0$. □



(a) (b)

Figure 7.1: Graph $\mathbb{G}$ of prismane C_8.

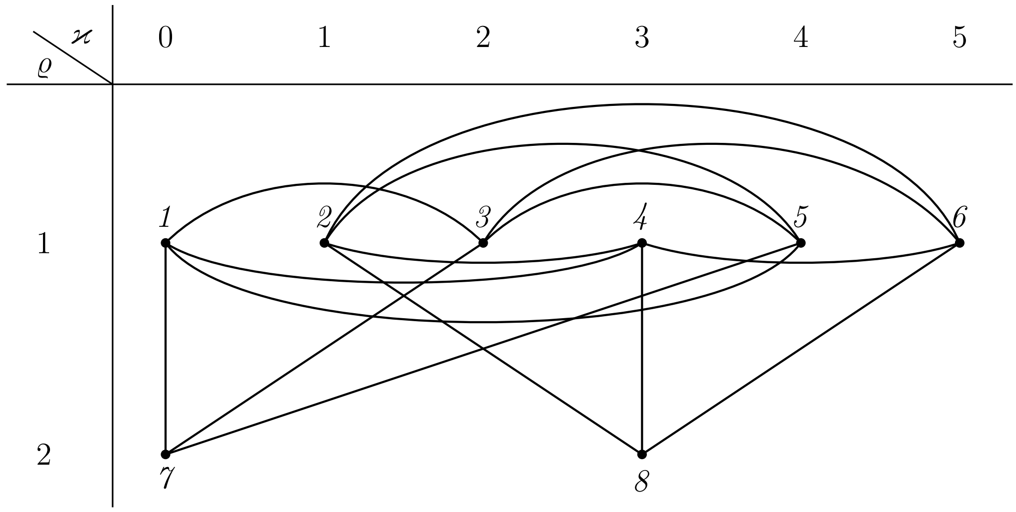


Figure 7.2: Graph $\mathbb{G}$ of prismane rearranged

7 Appendix: An Example

We consider the graph $\mathbb{G}$ of prismane C_8, a metastable carbon cluster analyzed in [4]; Figs. 7.1 both show this graph. From Fig. 7.1(b) we take that $P = (1\,2\,3\,4\,5\,6)(7\,8)$ is an automorphism of $\mathbb{G}$. In Fig. 7.2 graph $\mathbb{G}$ is rearranged according to this permutation. Fig. 7.3 shows the resulting graphs $\mathbb{G}(\varkappa)$ whose eigenvalues and eigenvectors determine those of $\mathbb{G}$ (Theorems 5.1, 5.2), see Fig. 7.4. From the complex eigenvectors we obtain real ones by taking the real and the imaginary parts. Note that the eigenvectors are pairwise orthogonal (Theorem 5.3).

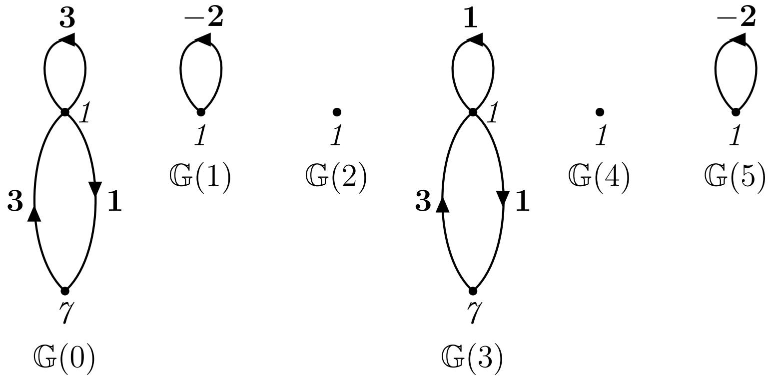


Figure 7.3: The graphs resulting from the reduction procedure as applied to the prismane graph $\mathbb{G}$.

Graph	**Eigen−values**	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*
$\mathbb{G}(0)$	α	1						$-\beta$	
	β	1						$-\alpha$	
$\mathbb{G}(1)$	-2	1							
$\mathbb{G}(2)$	0	1							
$\mathbb{G}(3)$	γ	1						$-\delta$	
	δ	1						$-\gamma$	
$\mathbb{G}(4)$	0	1							
$\mathbb{G}(5)$	-2	1							
$\mathbb{G}$	α	1	1	1	1	1	1	$-\beta$	$-\beta$
	β	1	1	1	1	1	1	$-\alpha$	$-\alpha$
	-2	1	η	η^2	η^3	η^4	η^5	0	0
	0	1	η^2	η^4	1	η^2	η^4	0	0
	γ	1	-1	1	-1	1	-1	$-\delta$	δ
	δ	1	-1	1	-1	1	-1	$-\gamma$	γ
	0	1	η^4	η^2	1	η^4	η^2	0	0
	-2	1	η^5	η^4	η^3	η^2	η	0	0

$$\alpha = \tfrac{1}{2}(3+\sqrt{21}) = 3,79\ldots \qquad \gamma = \tfrac{1}{2}(1+\sqrt{13}) = 2,30\ldots$$

$$\beta = \tfrac{1}{2}(3-\sqrt{21}) = -0,79\ldots \qquad \delta = \tfrac{1}{2}(1-\sqrt{13}) = -1,30\ldots$$

$$\eta = \exp(2\pi i/6) = \tfrac{1}{2} + \tfrac{i}{2}\sqrt{3}$$

Figure 7.4: Eigenvalues and eigenvectors of the prismane graph $\mathbb{G}$.

References

[1] Cvetković, D.M., Doob, M., Sachs, H., *Spectra of Graphs*, Deutscher Verlag der Wissenschaften, Berlin 1980/81; Academic Press, New York 1980; J.A. Barth Verlag, Heidelberg-Leipzig 1995.

[2] Davidson, R.A., *Spectral analysis of graphs by cyclic automorphism subgroups*. Theoret. Chim. Acta (Berl.) **58** (1981), 193–231.

[3] Dias, J.R., *Molecular Orbital Calculations Using Chemical Graph Theory.* Springer-Verlag, Berlin 1993.

[4] Elesin, V.F., Podlivaev, A.I., Openov, L.A., *Metastability of the three-dimensional carbon cluster Prismane* C_8*.* arXiv:physics/0104058v1 [physics.atm-clus] 19 Apr 2001.