

Nullity of a Graph with a Cut-Edge

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Abstract

The nullity of a graph is known to be an analytical tool to predict reactivity and conductivity of molecular π -systems. In this paper we consider the change in nullity when graphs with a cut-edge, and others derived from them, undergo geometrical operations. In particular, we consider the deletion of edges and vertices, the contraction of edges and the insertion of an edge at a coalescence vertex. We also derive three inequalities on the nullity of graphs along the same lines as the consequences of the Interlacing Theorem. These results shed light, in the tight-binding source and sink potential model, on the behaviour of molecular graphs which allow or bar conductivity in the cases when the connections are either distinct or ipso.

1 Introduction

Let G be a simple undirected graph with vertex set $\mathcal{V} = \mathcal{V}(G)$ and edge set $\mathcal{E} = \mathcal{E}(G)$. A graph F is a *subgraph* of G if $\mathcal{V}(F) \subseteq \mathcal{V}(G)$ and $\mathcal{E}(F) \subseteq \mathcal{E}(G)$. If $v \in \mathcal{V}(G)$ is deleted from G and the graph, $G - v$, obtained has more components than G , then v is a cut-vertex of G . Similarly, a cut-edge $e \in \mathcal{E}(G)$ is an edge whose deletion increases by one the number

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of components in the resulting graph $G - e$. Given two *component graphs* F_1 and F_2 , with root vertices v_1 and v_2 , respectively, the *coalescence* $G = F_1 \circ F_2$ is the graph obtained by identifying v_1 with v_2 , that is, these two vertices are replaced with a single vertex incident to all the edges which are incident to v_1 and v_2 in F_1 and F_2 , respectively. The vertex v in G formed by the identification of v_1 and v_2 is the *coalescence vertex* and it is a cut-vertex of the coalescence G .

The $n \times n$ *adjacency matrix* $\mathbf{A} = \mathbf{A}(G) = (a_{ij})$ of G encodes the adjacencies between the vertices of a labelled graph G on n vertices. The entry a_{ij} is one if there is an edge $e = v_i v_j$ between the vertices v_i and v_j , and zero otherwise. The *characteristic polynomial of the graph* G , denoted by $\phi(G)$, is the characteristic polynomial $\det(\lambda \mathbf{I} - \mathbf{A})$ of the adjacency matrix \mathbf{A} , where \mathbf{I} is the $n \times n$ identity matrix. If zero is an eigenvalue of \mathbf{A} , then \mathbf{A} is a singular matrix and the graph G is *singular*; otherwise G is *nonsingular*. The eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of \mathbf{A} are the *eigenvalues of the graph* G , and they form the *spectrum* of G . Since \mathbf{A} is a real symmetric matrix, its eigenvalues are real numbers. The *nullity* $\eta(G)$ is the multiplicity of the eigenvalue zero in the spectrum of the graph G . The *nullspace* of G is the eigenspace associated with the eigenvalue zero and a *kernel eigenvector* is a vector $\mathbf{x}(\neq \mathbf{0})$ in the nullspace $\ker(\mathbf{A})$ of \mathbf{A} .

In the sequel, we make use of the following two important results, namely Schwenk's Coalescence Theorem and a consequence of Cauchy's Interlacing Theorem for real symmetric matrices, respectively, stated hereunder for graphs in Theorems 1.1 and 1.2.

Theorem 1.1. [14] *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2 , respectively. The characteristic polynomial of the coalescence $H_1 \circ H_2$ is given by*

$$\phi(H_1 \circ H_2) = \phi(H_1)\phi(G_2) + \phi(G_1)\phi(H_2) - \lambda\phi(G_1)\phi(G_2).$$

Theorem 1.2. [11, pp.119] *Let u be any vertex of a graph G on $n \geq 2$ vertices. Then*

$$\eta(G) - 1 \leq \eta(G - u) \leq \eta(G) + 1.$$

The Interlacing Theorem permits the nullity of a graph to change by at most one upon the deletion or addition of a vertex. It admits three types of vertices; the first type is a *core vertex* (CV) u for which $\eta(G - u) = \eta(G) - 1$ [17]. In [18], it was shown that a necessary and sufficient condition for the nullity of a graph G to increase on the addition of a vertex u is that the vertex u is a CV. If $\eta(G - u)$ is either equal to $\eta(G)$ or to $\eta(G) + 1$,

then the vertex u is a *core-forbidden vertex* or, equivalently, a *Fiedler vertex*. Following the terminology used in [4], a vertex u is a *middle core-forbidden vertex* (CFV_{mid}) if $\eta(G - u) = \eta(G)$ and an *upper core-forbidden vertex* (CFV_{upp}) if $\eta(G - u) = \eta(G) + 1$. In the literature, vertices which are CFV_{upp} are also referred to as *Parter vertices* [10].

Almost 60 years ago, Collatz and Sinogowitz posed the problem of characterizing all singular graphs [2]. Significant progress in this regards was done in [6], [15] and [16]. However the problem is still not yet solved completely and research is ongoing. More recently, Ali *et al.* [1], determined the nullity of subgraphs obtained by perturbations of the coalescence G relative to the nullity of G .

The close link between the electron energy given by Schrödinger's equation in the quantum theory of molecules [8] and the nullity of a molecular graph was first recognised almost 60 years ago [5, 13]. A molecular graph is a labelled graph with vertices representing the atoms of a π -system and edges representing the chemical sigma bonds. The nullity of a molecular graph proved to be a predictive instrument in molecular reactivity and conductivity. For alternant unsaturated conjugated hydrocarbons, it gives an indication of the stability of the associated compound. An alternant unsaturated conjugated hydrocarbon with an unstable open-shell electron configuration corresponds to a singular bipartite graph. The associated compound is predicted to be so highly reactive that it decomposes as soon as it is formed. This prediction is significant in molecular orbital theory and it has been experimentally verified in numerous cases. For instance, there are more than a thousand stable benzenoid hydrocarbons whose molecular graphs are non-singular, whilst to date no stable benzenoid hydrocarbon whose molecular graph has a non-zero nullity is known [6].

More recently, the incessant activity focusing on carbon nano molecules and their conductivity properties has led to a better understanding of how these can be utilised in circuits as conductors or insulators of electric current. In particular, much research (see, for example, [3, 12, 19]) has been carried out to establish when a molecule, connected via two or one of its atoms in a circuit by two similar semi-infinite wires, allows or bars conductivity at the Fermi level (which corresponds to the zero energy level in the tight-binding source and sink potential model). The research distinguishes between the two setups that are possible, namely the *distinct connection* when two distinct atoms in the molecular graph act as the connecting vertices v_1 and v_2 , and the *ipso connection* when

there is only one connecting vertex ($v_1 = v_2$) for the two wires. In Theorem 4.3 of [3], it is demonstrated that when the distinct connecting vertices v_1 and v_2 are CV in a molecular graph G for which $\eta(G) \geq 2$, then conductivity does **not** occur if and only if v_1 and v_2 are also CV in $G - v_2$ and $G - v_1$, respectively. Furthermore, in Theorem 4.5 of [3], it is also shown that for an ipso connection, a singular molecular graph allows conductivity if and only if the connecting atom $v_1(= v_2)$ is either a CV or a CFV_{mid}.

Figure 1 illustrates the graph G with a cut-edge e and the subgraphs of G which are of interest to us in this work. For a graph G with a cut-edge $e = v_1v_2$, let $G - e$ be $F_1 \dot{\cup} F_2$, where $F_1 - v_1 = G_1 \dot{\cup} G_2 \dot{\cup} \dots \dot{\cup} G_r$ and $F_2 - v_2 = G_{r+1} \dot{\cup} G_{r+2} \dot{\cup} \dots \dot{\cup} G_s$, for $r \in \{1, \dots, s-1\}$. The coalescence $F_1 \circ K_2$ (or $F_1 + v_2$) of the graph F_1 and the complete graph K_2 has terminal vertex v_2 . Similarly $F_2 \circ K_2 = F_2 + v_1$ has terminal vertex v_1 . We remark that the two components of $G - e$ can be labelled F_1 and F_2 arbitrarily. Thus, when in the sequel we refer to F_1 , we implicitly imply that F_1 with root vertex v_1 is chosen without loss of generality from the two components of $G - e$. Also, if G is a graph with a cut-edge $e = v_1v_2$, a result obtained on the premise that v_1 is of a certain type in F_1 or in G will also hold, without loss of generality, if v_2 is of that same type in F_2 or in G . For an edge $e = v_1v_2$ of a graph G , the graph obtained from G by *contracting* the edge e to a new vertex v , such that v will be adjacent to all the (former) neighbours of v_1 and v_2 in G , is denoted by $\mathcal{G} = G/e$. We note that the graph G can be obtained back from \mathcal{G} by replacing the vertex v of \mathcal{G} by the edge $e = v_1v_2$ for a unique choice of the neighbours of v_1 and v_2 in G ; we write $G = \mathcal{G} : e$ (a formal discussion on this operation is presented in Section 6).

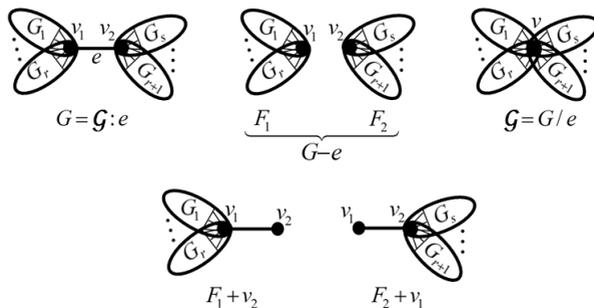


Figure 1. The graphs $G = \mathcal{G} : e$, $G - e = F_1 \dot{\cup} F_2$, $\mathcal{G} = G/e$, $F_1 + v_2$ and $F_2 + v_1$, where $e = v_1v_2$.

The rest of this paper is structured as follows. In Section 2, we consider graphs with a terminal vertex and discuss the type of this vertex and of its neighbour. For a graph G with a cut-edge e such that the components of $G - e$ are F_1 and F_2 , the properties of the end vertices of e are used to prove our main results, namely:

- (i) the types of the end vertices of the cut-edge e in G are determined, given their types as root vertices in F_1 and F_2 (Section 3);
- (ii) the difference in nullity $\eta(G - e) - \eta(G)$ is restricted to the range -1 to 2 for a cut-edge e (Section 4);
- (iii) if the cut-edge e is contracted, then the difference in the nullity of G and of G/e is at most one (Section 5);
- (iv) if a cut-vertex of G is replaced by a cut-edge, the nullity changes by at most one (Section 6).

The results stated above have important implications in both the distinct and ipso connections in electrical circuits. We show that:

- (i) for a *distinct connection*, conductivity necessarily occurs if the connecting vertices v_1 and v_2 which are the end-vertices of a cut-edge in a molecular graph, are both CV (Theorem 3.11); and
- (ii) for an *ipso connection* at a cut-vertex v in a molecular graph G , which is obtained from a graph of nullity at least two by contracting a cut-edge joining a CFV_{upp} with a CV to v , the molecule G is an insulator (Corollary 5.3).

2 Graphs with a terminal vertex

We start this section by discussing the type of the neighbour of a terminal vertex in a graph. Let F_1 be a graph with root vertex v_1 and let v_2 be the terminal vertex of $F_1 + v_2$, where v_1v_2 is a pendant edge. The following well-known result appears in [20].

Lemma 2.1. [20] *The nullity remains unchanged when the two vertices incident to a pendant edge are deleted.*

An immediate consequence is that the type of neighbour of a terminal vertex is determined uniquely, independent of the type of the terminal vertex. However, as we show in Theorems 2.4, 2.5 and 2.6, the terminal vertex may be of any type.

Lemma 2.2. *In $F_1 + v_2$, the vertex v_1 is a CFV_{upp} .*

Proof. Let $L = F_1 + v_2$. Since v_2 is a terminal vertex and $L - v_1 = (L - \{v_1, v_2\}) \dot{\cup} K_1$, then $\eta(L - v_1) = \eta(L - \{v_1, v_2\}) + 1$. By Lemma 2.1, $\eta(L) = \eta(L - \{v_1, v_2\})$ and thus $\eta(L - v_1) = \eta(L) + 1$. By definition, v_1 is a CFV_{upp} in L . ■

In the rest of this section, we determine the type of the terminal vertex v_2 in $F_1 + v_2$ by exploring the possible types of v_1 in F_1 . Since the proofs make use of the coalescence $F_1 \circ K_2$, we need the following results from [1].

Theorem 2.3. [1] *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2 , respectively, and let H be the coalescence of H_1 and H_2 obtained by identifying the vertices v_1 and v_2 to get the coalescence vertex v .*

- (i) *If v_1 is a CV in H_1 or v_2 is a CV in H_2 , then $\eta(H) = \eta(H_1) + \eta(H_2) - 1$.*
- (ii) *If v_1 is a CFV_{upp} in H_1 and v_2 is a CFV_{mid} in H_2 , then $\eta(H) = \eta(H_1) + \eta(H_2)$.*
- (iii) *If each of v_1 and v_2 is a CFV_{upp} in the respective component graph, then $\eta(H) = \eta(H_1) + \eta(H_2) + 1$.*
- (iv) *If each of v_1 and v_2 is a CFV_{mid} in the respective component graph, then either v is a CFV_{mid} in H and $\eta(H) = \eta(H_1) + \eta(H_2)$, or v is a CV in H and $\eta(H) = \eta(H_1) + \eta(H_2) + 1$.*

In Theorem 2.4 we consider $F_1 + v_2$ when v_1 is a CV in F_1 .

Theorem 2.4. *Let F_1 be a graph with root vertex v_1 , and let $F_1 + v_2$ be obtained from F_1 by joining a new vertex v_2 to v_1 by an edge. Then v_1 is a CV in F_1 if and only if v_2 is a CFV_{upp} in $F_1 + v_2$.*

Proof. Since each vertex of K_2 is a CFV_{upp} in K_2 , if v_1 is a CV in F_1 , then by Theorem 2.3(i), $\eta(F_1 + v_2) = \eta(F_1) + \eta(K_2) - 1$. But $\eta(K_2) = 0$; thus $\eta(F_1 + v_2) = \eta(F_1) - 1$. Hence, v_2 is a CFV_{upp} in $F_1 + v_2$.

Conversely, let v_2 be a CFV_{upp} in $F_1 + v_2$. By definition, $\eta(F_1) = \eta(F_1 + v_2) + 1$. By Lemma 2.1, $\eta(F_1 + v_2) = \eta(F_1 - v_1)$, implying that $\eta(F_1 - v_1) = \eta(F_1) - 1$. Hence, v_1 is a CV in F_1 . ■

The case when v_1 is a CFV_{mid} in F_1 is considered in Theorem 2.5.

Theorem 2.5. *Let F_1 be a graph with root vertex v_1 , and let $F_1 + v_2$ be obtained from F_1 by joining a new vertex v_2 to v_1 by an edge. Then v_1 is a CFV_{mid} in F_1 if and only if v_2 is a CFV_{mid} in $F_1 + v_2$.*

Proof. If v_1 is a CFV_{mid} in F_1 , then by Theorem 2.3(ii), $\eta(F_1 + v_2) = \eta(F_1) + \eta(K_2)$. It follows that $\eta(F_1 + v_2) = \eta(F_1)$. Hence, v_2 is a CFV_{mid} in $F_1 + v_2$.

Conversely, let v_2 be a CFV_{mid} in $F_1 + v_2$. Thus, $\eta(F_1 + v_2) = \eta(F_1)$. By Lemma 2.1, $\eta(F_1 + v_2) = \eta(F_1 - v_1)$, implying that $\eta(F_1) = \eta(F_1 - v_1)$. Hence, v_1 is a CFV_{mid} in F_1 . ■

The case when v_1 is a CFV_{upp} in F_1 follows by exclusion, from all the possible cases, of the occurrences mentioned in Theorems 2.4 and 2.5.

Theorem 2.6. *Let F_1 be a graph with root vertex v_1 , and let $F_1 + v_2$ be obtained from F_1 by joining a new vertex v_2 to the v_1 by an edge. Then v_1 is a CFV_{upp} in F_1 if and only if v_2 is a CV in $F_1 + v_2$.*

We have shown that by knowing the type of the root vertex v_1 in F_1 , we can immediately deduce the type of the terminal vertex v_2 in $F_1 + v_2$, and conversely. Table 1 illustrates this bijective relationship. A clear dichotomy appears between the type CFV_{mid} and the other two types of vertices.

v_1 in F_1	v_2 in $F_1 + v_2$
CFV_{upp}	CV
CV	CFV_{upp}
CFV_{mid}	CFV_{mid}

Table 1. The type of a terminal vertex.

3 Type of vertices incident to a cut-edge

Heilbronner [7] obtained the characteristic polynomial of a graph G having a cut-edge by applying the Laplacian development to the determinant $\phi(G)$. The result is given here in Theorem 3.1. We adopt an algebraic-geometric approach by constructing G as a coalescence to give a different (much simpler) proof from the one given by Heilbronner.

Theorem 3.1. [7] *The characteristic polynomial of a graph G with a cut-edge $e = v_1v_2$ is given as: $\phi(G) = \phi(G - e) - \phi(G - \{v_1, v_2\})$.*

Proof. Let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. Recall that the characteristic polynomials of the complete graphs K_1 and K_2 on one and two vertices are λ and $\lambda^2 - 1$, respectively. By Theorem 1.1, we have $\phi(F_1 + v_2) = \lambda\phi(F_1) - \phi(F_1 - v_1)$. Now, $F_1 + v_2$ is a graph with root vertex v_2 . Applying Theorem 1.1 again to determine the characteristic polynomial of the graph $G = (F_1 + v_2) \circ F_2$, we have

$$\begin{aligned} \phi(G) &= \phi(F_1 + v_2)\phi(F_2 - v_2) + \phi(F_1)\phi(F_2) - \lambda\phi(F_1)\phi(F_2 - v_2) \\ &= (\lambda\phi(F_1) - \phi(F_1 - v_1))\phi(F_2 - v_2) + \phi(F_1)\phi(F_2) - \lambda\phi(F_1)\phi(F_2 - v_2) \\ &= \phi(F_1)\phi(F_2) - \phi(F_1 - v_1)\phi(F_2 - v_2) \\ &= \phi(G - e) - \phi(G - \{v_1, v_2\}). \end{aligned}$$

■

In the rest of this section, we determine the type of the vertex v_1 incident to a cut-edge $e = v_1v_2$ in a graph G , given the type of the root vertex v_1 in the component graph F_1 or $F_2 + v_1$. We require the following results from [1].

Theorem 3.2. [1] *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2 , respectively, and let H be the coalescence of H_1 and H_2 obtained by identifying the vertices v_1 and v_2 to get the coalescence vertex v .*

- (i) *If v_1 is a CFV_{upp} in H_1 or v_2 is a CFV_{upp} in H_2 , then v is a CFV_{upp} in H .*
- (ii) *If each of v_1 and v_2 is a CV in the respective component graph, then v is a CV in H .*
- (iii) *If v_1 is a CV in H_1 and v_2 is a CFV_{mid} in H_2 , then v is a CFV_{mid} in H .*
- (iv) *If each of v_1 and v_2 is a CFV_{mid} in the respective component graph, then v is either a CFV_{mid} or a CV in H .*

Since the graph G with a cut-edge $e = v_1v_2$ is obtained from the coalescence of the component graphs F_1 and $F_2 + v_1$, each having root vertex v_1 , by using Theorem 3.2, we can deduce the following result.

Theorem 3.3. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively.*

- (i) *If v_1 is a CFV_{upp} in F_1 or in $F_2 + v_1$, then v_1 is a CFV_{upp} in G .*
- (ii) *If v_1 is a CV in each of F_1 and $F_2 + v_1$, then v_1 is a CV in G .*

- (iii) If v_1 is a CV in F_1 and a CFV_{mid} in $F_2 + v_1$, or if v_1 is a CFV_{mid} in F_1 and a CV in $F_2 + v_1$, then v_1 is a CFV_{mid} in G .
- (iv) If v_1 is a CFV_{mid} in each of F_1 and $F_2 + v_1$, then v_1 is either a CFV_{mid} or a CV in G .

The following result is immediate from Theorems 2.4 and 3.3(i).

Theorem 3.4. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. If v_1 is a CV in F_1 , then v_2 is a CFV_{upp} in G .*

Note that this result is independent of the type of v_2 in F_2 . Theorem 3.5 deals with the instance when v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 .

Theorem 3.5. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. If v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 , then v_1 is a CFV_{mid} and v_2 is a CFV_{upp} in G .*

Proof. Since v_1 is a CV in F_1 , then by Theorem 3.4, v_2 is a CFV_{upp} in G . By Theorem 2.5, since v_2 is a CFV_{mid} in F_2 , then v_1 is also a CFV_{mid} in $F_2 + v_1$. Thus, by Theorem 3.3(iii), v_1 is a CFV_{mid} in G . ■

If we know that at least one of the root vertices of F_1 and F_2 is a CFV_{upp}, then we are able to determine the type of both v_1 and v_2 in G . This is the result of Theorem 3.6.

Theorem 3.6. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. If v_1 is a CFV_{upp} in F_1 , then the type of each of v_1 and v_2 remains unchanged in G .*

Proof. Since v_1 is a CFV_{upp} in F_1 , by Theorem 3.3(i), v_1 is a CFV_{upp} in G and by Theorem 2.6, v_2 is a CV in $F_1 + v_2$. Now, G is obtained by identifying the vertex v_2 in $F_1 + v_2$ with the vertex v_2 in F_2 . We consider the three different cases for the type of v_2 in F_2 .

- (i) If v_2 is a CFV_{upp} in F_2 , then by Theorem 3.2(i), v_2 is a CFV_{upp} in G .
- (ii) If v_2 is a CV in F_2 , then by Theorem 3.2(ii), v_2 is a CV in G .
- (iii) If v_2 is a CFV_{mid} in F_2 , then by Theorem 3.2(iii), v_2 is a CFV_{mid} in G .

Hence, v_1 and v_2 remain of the same type in G . ■

The case when the two root vertices are of the same type in F_1 and F_2 is presented in Theorem 3.7.

Theorem 3.7. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively.*

- (i) *If each of v_1 and v_2 is a CV in F_1 and F_2 , respectively, then each of v_1 and v_2 is a CFV_{upp} in G .*
- (ii) *If each of v_1 and v_2 is a CFV_{upp} in F_1 and F_2 , respectively, then each of v_1 and v_2 is a CFV_{upp} in G .*
- (iii) *If each of v_1 and v_2 is a CFV_{mid} in F_1 and F_2 , respectively, then v_1 and v_2 are either both CV or both CFV_{mid} in G .*

Proof. We note that (i) and (ii) are special cases of Theorem 3.4 and Theorem 3.6, respectively.

To prove (iii), note that $\eta(G - v_1) = \eta(F_1 - v_1) + \eta(F_2)$ (refer to Figure 1). Since v_2 is a CFV_{mid} in F_2 , then $\eta(G - v_1) = \eta(F_1 - v_1) + \eta(F_2 - v_2)$. Similarly, since v_1 is a CFV_{mid} in F_1 , then $\eta(G - v_2) = \eta(F_1 - v_1) + \eta(F_2 - v_2)$. Also, $\eta(G - v_1) = \eta(G - v_2)$. We conclude that v_1 and v_2 are of the same type in G . Moreover, by Theorems 2.5 and 3.3(iv), v_1 and v_2 cannot be CFV_{upp} in G . ■

Table 2 illustrates all the possible cases. Further to the relationship among the types of vertices presented in Table 1, we note that the type of v_1 and v_2 in G is determined uniquely by knowing the type of v_1 in F_1 and the type of v_2 in F_2 , except for the instance when the root vertices v_1 and v_2 are both CFV_{mid} in F_1 and F_2 .

v_1 in F_1	v_2 in F_2	v_1 in G	v_2 in G
CFV_{upp}	CFV_{upp}	CFV_{upp}	CFV_{upp}
CFV_{upp}	CV	CFV_{upp}	CV
CFV_{upp}	CFV_{mid}	CFV_{upp}	CFV_{mid}
CV	CV	CFV_{upp}	CFV_{upp}
CV	CFV_{mid}	CFV_{mid}	CFV_{upp}
CFV_{mid}	CFV_{mid}	CFV_{mid}	CFV_{mid}
		CV	CV

Table 2. Type of the vertices incident to a cut-edge $e = v_1v_2$.

After considering all the possible types of pairs of vertices, the following result follows immediately.

Theorem 3.8. *It is impossible to have a graph G with a cut-edge $e = v_1v_2$ such that v_1 is a CFV_{mid} and v_2 is a CV in G .*

The case when v_1 and v_2 are both CV in G has an interesting consequence on one of the kernel eigenvectors of G , as follows.

Theorem 3.9. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. If v_1 and v_2 are both CV in G , then*

- (i) *each of v_1 and v_2 is a CFV_{mid} in F_1 and F_2 , respectively;*
- (ii) *v_1 and v_2 correspond to non-zero entries on exactly one kernel eigenvector in a basis for the nullspace of $\mathbf{A}(G)$.*

Proof. From Table 2, v_1 and v_2 are both CV in G if they are both CFV_{mid} in F_1 and F_2 , respectively; hence (i) follows immediately. To prove (ii), let $\eta(G) = \eta$ and let both v_1 and v_2 be CV in G . Then there exist kernel eigenvectors with a non zero entry at the positions corresponding to v_1 and v_2 . Let $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(\eta-1)}$ be linearly independent kernel eigenvectors in the nullspace of $\mathbf{A}(G)$ with a zero entry at the position corresponding to the vertex v_1 , and let $\mathbf{x}^{(\eta)}$ be a kernel eigenvector having a non zero entry at that position. Note that if $\mathbf{x}_{\text{res.}}^{(i)}$ is the vector obtained from $\mathbf{x}^{(i)}$ by removing the zero entry at the position corresponding to v_1 , thus reducing its dimension by one, then $\mathbf{x}_{\text{res.}}^{(i)}$ is a kernel eigenvector of $\mathbf{A}(G - v_1)$. Since $\eta(G - v_1) = \eta - 1$, then $\mathbf{x}_{\text{res.}}^{(1)}, \mathbf{x}_{\text{res.}}^{(2)}, \dots, \mathbf{x}_{\text{res.}}^{(\eta-1)}$ are $\eta - 1$ linearly independent eigenvectors generating the nullspace of $\mathbf{A}(G - v_1)$. Suppose there is some $\mathbf{x}_{\text{res.}}^{(i)}$, for $i \in \{1, 2, \dots, \eta - 1\}$, having a non zero entry at the position corresponding to the vertex v_2 . Since v_2 is a CV in G , then $G - \{v_1, v_2\}$ has nullity

$$\eta(G - \{v_1, v_2\}) = \eta(G - v_1) - 1 = \eta - 2. \tag{1}$$

However, $\eta(G - \{v_1, v_2\}) = \eta(F_1 - v_1) + \eta(F_2 - v_2)$ and from the proof of Theorem 3.7(iii), $\eta(F_1 - v_1) + \eta(F_2 - v_2) = \eta(G - v_1) = \eta(G - v_2)$. Thus, $\eta(G - \{v_1, v_2\}) = \eta - 1$, a contradiction to (1). Hence the kernel eigenvector containing the non zero entry at the position corresponding to the vertex v_1 must also contain the non zero entry at the

position corresponding to the vertex v_2 . Thus, each of $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(\eta-1)}$ has a zero entry at both positions corresponding to the vertices v_1 and v_2 , implying that if v_1 and v_2 are CV in G then they correspond to non-zero entries on the same kernel eigenvector in the nullspace of $\mathbf{A}(G)$. Indeed, on deleting both vertices, the nullity reduces by one only. Hence, there is one and only one kernel eigenvector (up to multiplicities) that has non-zero entries in these positions. ■

We conclude this section by presenting a chemical application of Theorem 3.9 by proving a sufficient condition for a molecular graph with a cut-edge to be an insulator. We first extract the following result from Table III of [3].

Lemma 3.10. [3] *Let G be a molecular graph with two distinct core vertices v_1 and v_2 . Then G with connecting vertices v_1 and v_2 is an insulator if and only if $\eta(G - \{v_1, v_2\}) = \eta(G) - 2$.*

We thus have the following result.

Theorem 3.11. *A molecular graph G with a cut-edge whose end vertices v_1 and v_2 are the connecting vertices of a molecule in a circuit cannot be an insulator if v_1 and v_2 are both CV in G .*

Proof. By Theorem 3.9, v_1 and v_2 correspond to non-zero entries on one kernel eigenvector only, and thus $\eta(G - \{v_1, v_2\}) = \eta(G) - 1$. Hence, from Lemma 3.10, G is not an insulator. ■

4 Nullity of graphs with a cut-edge

In [9], Ibrahim remarked that the nullity of a graph changes by at most two upon deleting an edge. In Theorem 4.1, we present a short proof for this statement. We proceed to show, in Theorem 4.7, that the range can be restricted further when e is a cut-edge.

Theorem 4.1. *Let G be any non-empty graph, then for each $e \in E(G)$, $|\eta(G) - \eta(G - e)| \leq 2$.*

Proof. Let $e = v_1v_2$. By Theorem 1.2, $\eta(G) - 1 \leq \eta(G - v_1) \leq \eta(G) + 1$. We obtain $G - v_1 + v'$ by introducing a new vertex v' in $G - v_1$ adjacent to the same neighbours of v_1

in G excluding v_2 . Using Theorem 1.2 once again, we obtain $\eta(G) - 2 \leq \eta(G - v_1 + v') \leq \eta(G) + 2$. The result follows by noting that $G - v_1 + v' = G - e$. ■

Table 3 illustrates the statement of Theorem 4.1. It shows that the difference $\eta(G) - \eta(G - e)$ is realizable for all values between -2 and 2 . No example is exhibited in the case when $\eta(G) - \eta(G - e) = 2$ and e is a cut-edge in G because, as we shall have occasion to show in Theorem 4.7, no such graphs exist.

$\eta(G) - \eta(G - e)$	G	$\eta(G)$	$G - e$	$\eta(G - e)$
-2		1		3
		2		4
-1		1		2
		1		2
0		1		1
		1		1
1		2		1
		2		1
2		3		1

Table 3. The nullity of graphs and their subgraphs upon deleting an edge (cut-edge).

Given the type of vertex v_1 in the component graphs F_1 or $F_2 + v_1$, we are now in a position to determine the difference between the nullity of a graph G with a cut-edge e and the nullity of $G - e$. We use some further results from [1].

Theorem 4.2. [1] *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2 , respectively, and let H be the coalescence of H_1 and H_2 obtained by identifying the vertices v_1 and v_2 to get the coalescence vertex v .*

- (i) *If v_1 is a CFV_{upp} in H_1 , then $\eta(H) = \eta(H_1) + \eta(G_2) = \eta(H_1) + \eta(H_2 - v_2)$.*

(ii) If v_1 is a CV in H_1 , then $\eta(H) = \eta(G_1) + \eta(H_2) = \eta(H_1 - v_1) + \eta(H_2)$.

Again, we consider $G = F_1 \circ (F_2 + v_1)$ with coalescence vertex v_1 . If v_1 is a CFV_{upp} in F_1 , then by Theorem 4.2(i), $\eta(G) = \eta(F_1) + \eta(F_2) = \eta(G - e)$. Hence we have the following result.

Theorem 4.3. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively. If v_1 is a CFV_{upp} in F_1 , then $\eta(G) = \eta(G - e)$.*

Theorem 4.3 implies that if we know that at least one of the root vertices in F_1 and F_2 is a CFV_{upp} , then the nullity of $G - e$ is not influenced by the type of the other root vertex. The situation is completely different when none of the root vertices is a CFV_{upp} because the nullity will change on deleting e from G .

The case when one of the root vertices is a CV and the other is **not** a CFV_{upp} in the respective component graph is treated in Theorem 4.4.

Theorem 4.4. *Let G be a graph with a cut-edge $e = v_1v_2$ and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively.*

(i) *If each of v_1 and v_2 is a CV in F_1 and F_2 , respectively, then $\eta(G) = \eta(G - e) - 2$.*

(ii) *If v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 , then $\eta(G) = \eta(G - e) - 1$.*

Proof. Since v_1 is a CV in F_1 , by Theorem 4.2(ii), $\eta(G) = \eta(F_1 - v_1) + \eta(F_2 + v_1)$. By Lemma 2.1, $\eta(F_2 + v_1) = \eta(F_2 - v_2)$, and thus

$$\eta(G) = \eta(F_1 - v_1) + \eta(F_2 - v_2). \tag{2}$$

(i) Since v_1 and v_2 are both CV in F_1 and F_2 , respectively, then $\eta(F_1) = \eta(F_1 - v_1) + 1$ and $\eta(F_2) = \eta(F_2 - v_2) + 1$. Hence, by (2) we obtain $\eta(G) = \eta(F_1) - 1 + \eta(F_2) - 1 = \eta(G - e) - 2$.

(ii) Since v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 , then $\eta(F_1) = \eta(F_1 - v_1) + 1$ and $\eta(F_2) = \eta(F_2 - v_2)$. From (2), we obtain $\eta(G) = \eta(G - e) - 1$.

■

The following corollary is immediate from Theorems 2.4 and 4.4.

Corollary 4.5. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively.*

- (i) *If each of v_1 and v_2 is a CFV_{upp} in $F_2 + v_1$ and $F_1 + v_2$, respectively, then $\eta(G) = \eta(G - e) - 2$.*
- (ii) *If v_1 is a CFV_{upp} in $F_2 + v_1$ and a CFV_{mid} in F_1 , or if v_1 is a CFV_{mid} in $F_2 + v_1$ and a CFV_{upp} in F_1 , then $\eta(G) = \eta(G - e) - 1$.*

Proof. By Theorem 2.4, the vertex v_1 is a CFV_{upp} in $F_2 + v_1$ if and only if v_2 is a CV in F_2 , and v_2 is a CFV_{upp} in $F_1 + v_2$ if and only if v_1 is a CV in F_1 . Hence the result follows by Theorem 4.4. ■

Finally, to address the case when v_1 is a CFV_{mid} in F_1 , we need to consider the types of the vertex v_1 in G , as follows.

Theorem 4.6. *Let G be a graph with a cut-edge $e = v_1v_2$, and let F_1 and F_2 be the components of $G - e$ with root vertices v_1 and v_2 , respectively.*

- (i) *If v_1 is a CFV_{mid} in F_1 and a CFV_{upp} in G , then $\eta(G) = \eta(G - e) - 1$.*
- (ii) *If v_1 is a CFV_{mid} in F_1 and a CV in G , then $\eta(G) = \eta(G - e) + 1$.*
- (iii) *If v_1 is a CFV_{mid} in F_1 and a CFV_{mid} in G , then $\eta(G) = \eta(G - e)$.*

Proof.

- (i) Since v_1 is a CFV_{upp} in G , then by definition, $\eta(G) = \eta(G - v_1) - 1$. As shown in Figure 1, $G - v_1 = F_1 - v_1 \dot{\cup} F_2$, and thus $\eta(G - v_1) = \eta(F_1 - v_1) + \eta(F_2)$. Since, v_1 is a CFV_{mid} in F_1 , by definition, $\eta(G - v_1) = \eta(F_1) + \eta(F_2) = \eta(G - e)$. Hence, $\eta(G) = \eta(G - e) - 1$.
- (ii) Since v_1 is a CV in G , then $\eta(G) = \eta(G - v_1) + 1$. Since $G - v_1 = F_1 - v_1 \dot{\cup} F_2$ then $\eta(G - v_1) = \eta(F_1 - v_1) + \eta(F_2)$. Now, v_1 is a CFV_{mid} in F_1 and, by definition, $\eta(F_1 - v_1) = \eta(F_1)$. Thus $\eta(G - v_1) = \eta(F_1) + \eta(F_2)$ and hence $\eta(G) = \eta(F_1) + \eta(F_2) + 1 = \eta(G - e) + 1$.
- (iii) Since $G - v_1 = F_1 - v_1 \dot{\cup} F_2$, then $\eta(G - v_1) = \eta(F_1 - v_1) + \eta(F_2)$. Now, v_1 is a CFV_{mid} in F_1 , implying that $\eta(G - v_1) = \eta(F_1) + \eta(F_2) = \eta(G - e)$. Since v_1 is a CFV_{mid} in G , by definition we also have $\eta(G) = \eta(G - v_1)$. Hence, $\eta(G) = \eta(G - e)$. ■

At this point, we are able to prove our claim that there is no graph G with a cut-edge e such that $\eta(G) - \eta(G - e) = 2$.

Theorem 4.7. *If G is any graph with a cut-edge $e = v_1v_2$, then $\eta(G) - 1 \leq \eta(G - e) \leq \eta(G) + 2$.*

Proof. We consider all the six different possible cases for the type of vertex v_1 in F_1 and v_2 in F_2 .

- If either v_1 is a CFV_{upp} in F_1 or v_2 is a CFV_{upp} in F_2 , then by Theorem 4.3, $\eta(G) = \eta(G - e)$.
- If each of v_1 and v_2 is a CV in F_1 and F_2 , respectively, then by Theorem 4.4(i), $\eta(G) = \eta(G - e) - 2$.
- If either v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 , or v_1 is a CFV_{mid} in F_1 and v_2 is a CV in F_2 , then by Theorem 4.4(ii), $\eta(G) = \eta(G - e) - 1$.
- If each of v_1 and v_2 is a CFV_{mid} in F_1 and F_2 , respectively, then by Theorem 3.7(iii), v_1 and v_2 are either both CV or both CFV_{mid} in G . If they are both CV in G , then by Theorem 4.6(ii), $\eta(G) = \eta(G - e) + 1$; whilst if they are both CFV_{mid} in G , then by Theorem 4.6(iii), $\eta(G) = \eta(G - e)$.

Hence, in all possible cases, the nullity upon removing a cut-edge e from G lies between $\eta(G) - 1$ and $\eta(G) + 2$. ■

5 Contracting a cut-edge of a graph

In this section we show that on contracting a cut-edge, the nullity changes by at most one. In the following theorem, we first establish the type of the new vertex obtained upon contracting a cut-edge and derive the nullity of the resulting graph. The proof follows in two steps. We first delete the cut-edge to obtain two component graphs F_1 and F_2 with root vertices v_1 and v_2 , respectively, and use the results in Sections 3 and 4 to determine the nullity of the graph obtained and the type of the root vertices in F_1 and in F_2 . The second step involves coalescing the two component graphs using results from [1], presented here in Theorems 2.3 and 3.2. Thus we have:

Theorem 5.1. *Let G be a graph with a cut-edge $e = v_1v_2$, and let G/e be the graph G with the edge e contracted to the vertex v .*

- (i) If v_1 and v_2 are both CFV_{upp} in G , then v is either a CFV_{upp} or a CV in G/e and $\eta(G/e) = \eta(G) + 1$.
- (ii) If v_1 is a CFV_{upp} in G and v_2 is a CV in G , then v is a CFV_{upp} in G/e and $\eta(G/e) = \eta(G) - 1$.
- (iii) If v_1 is a CFV_{upp} in G and v_2 is a CFV_{mid} in G , then v is either a CFV_{upp} or a CFV_{mid} in G/e and $\eta(G/e) = \eta(G)$.
- (iv) If v_1 and v_2 are both CFV_{mid} in G , then either v is a CFV_{mid} in G/e and $\eta(G/e) = \eta(G)$, or v is a CV in G/e and $\eta(G/e) = \eta(G) + 1$.
- (v) If v_1 and v_2 are both CV in G , then either v is a CFV_{mid} in G/e and $\eta(G/e) = \eta(G) - 1$, or v is a CV in G/e and $\eta(G/e) = \eta(G)$.

We note that in Theorem 5.1, we do not consider the case when v_1 is a CFV_{mid} and v_2 is a CV in G because, as we discussed in Theorem 3.8, this case cannot occur.

Remark 5.2. *We have examples illustrating all the above situations except for the last case, that is, when v_1 and v_2 are both CV in G and v is a CV in G/e . We think that this case is not possible, but have no proof of this claim.*

In Theorem 4.5 of [3], it is proved that for an ipso connection, a singular molecular graph allows conductivity if and only if the connecting atom is either a CV or a CFV_{mid} . A consequence of Theorem 5.1 is the following chemical application to molecular graphs.

Corollary 5.3. *Let G be a graph of nullity at least two with a cut-edge e such that one of the end-vertices of e is a CFV_{upp} and the other end-vertex is a CV. A molecular graph obtained from G by contracting e to a vertex v is an insulator if the ipso connection is made at v .*

Along the same lines as the consequences of the Interlacing Theorem when a vertex is deleted, we state the next result for edge contraction which is another immediate consequence of Theorem 5.1.

Theorem 5.4. *Let G be a graph with a cut-edge e , and let G/e be the graph G with the edge e contracted to the vertex v . Then*

$$\eta(G) - 1 \leq \eta(G/e) \leq \eta(G) + 1.$$

6 Replacing a cut-vertex with an edge

In this section, we discuss the inverse to the problem discussed in Section 5. The coalescence $F_1 \circ F_2$, denoted by \mathcal{G} , is the graph with a cut-vertex $v = v_1 = v_2$ such that $\mathcal{G} - v = (F_1 - v_1) \dot{\cup} (F_2 - v_2)$. Recall that $F_1 - v_1 = \{G_1, \dots, G_r\}$ and $F_2 - v_2 = \{G_{r+1}, \dots, G_s\}$ for some $r \in \{1, \dots, s-1\}$. The graph $\mathcal{G} : e$ is constructed by introducing the edge $e = v_1 v_2$ in $F_1 \dot{\cup} F_2$. Note that $\mathcal{G} : e$ is identical to the graph G with cut-edge $v_1 v_2$.

The following theorem follows immediately from Theorem 5.1.

Theorem 6.1. *Let v be a cut-vertex in \mathcal{G} and let $e = v_1 v_2$ in $\mathcal{G} : e$.*

1. *If v is a CFV_{upp} in \mathcal{G} , then v_1 or v_2 is a CFV_{upp} in $\mathcal{G} : e$.*
2. *If v is a CV in \mathcal{G} , then v_1 and v_2 are of the same type (either both CFV_{upp} or both CV or both CFV_{mid}) in $\mathcal{G} : e$.*
3. *If v is a CFV_{mid} in \mathcal{G} , then in $\mathcal{G} : e$, either*
 - (i) *v_1 and v_2 are both CV, or*
 - (ii) *v_1 and v_2 are both CFV_{mid} , or*
 - (iii) *v_1 is a CFV_{mid} and v_2 is a CFV_{upp} , or v_1 is a CFV_{upp} and v_2 is a CFV_{mid} .*

As we noted in Remark 5.2, we know of no graph \mathcal{G} in which v is a CV such that both vertices v_1 and v_2 are CV in $\mathcal{G} : e$.

In Theorems 6.3 to 6.5, we use the type of the cut-vertex v in \mathcal{G} to determine the nullity of the graph $\mathcal{G} : e$. For this purpose we need three results from [1], stated here in Theorem 6.2.

Theorem 6.2. [1] *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two component graphs with root vertices v_1 and v_2 , respectively, that form the coalescence G obtained by identifying the vertices v_1 and v_2 to get the coalescence vertex v .*

- (i) *If v is a CV in G , then v_1 and v_2 are either both CV or both CFV_{mid} in H_1 and H_2 .*
- (ii) *The vertex v is a CFV_{upp} in G if and only if at least one of v_1 and v_2 is a CFV_{upp} in H_1 or H_2 .*
- (iii) *If v is a CFV_{mid} in G , then either v_1 and v_2 are both CFV_{mid} in H_1 and H_2 , or v_1 is a CFV_{mid} in H_1 and v_2 is a CV in H_2 .*

Theorem 6.3. *Let \mathcal{G} be a graph with a cut-vertex v . If v is a CFV_{upp} in \mathcal{G} , then $\eta(\mathcal{G}) - 1 \leq \eta(\mathcal{G} : e) \leq \eta(\mathcal{G}) + 1$.*

Proof. Since v is a CFV_{upp} in \mathcal{G} , by Theorem 6.2(ii), either v_1 is a CFV_{upp} in F_1 or v_2 is a CFV_{upp} in F_2 , and by Theorem 4.3, since $G = \mathcal{G} : e$, $\eta(G - e) = \eta(\mathcal{G} : e)$. We have three cases to consider.

- (i) If v_1 and v_2 are both CFV_{upp} in F_1 and F_2 , respectively, then by Theorem 2.3(iii), $\eta(\mathcal{G}) = \eta(G - e) + 1$, and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G}) - 1$.
- (ii) If v_1 is a CFV_{upp} in F_1 and v_2 is a CFV_{mid} in F_2 , then by Theorem 2.3(ii), $\eta(\mathcal{G}) = \eta(G - e)$, and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G})$.
- (iii) If v_1 is a CFV_{upp} in F_1 and v_2 is a CV in F_2 , then by Theorem 2.3(i), $\eta(\mathcal{G}) = \eta(G - e) - 1$, and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G}) + 1$.

■

Theorem 6.4. *Let \mathcal{G} be a graph with a cut-vertex v . If v is a CV in \mathcal{G} , then $\eta(\mathcal{G} : e)$ is either $\eta(\mathcal{G}) - 1$ or $\eta(\mathcal{G})$.*

Proof. Since v is a CV in \mathcal{G} , then by Theorem 6.2(i) we have two cases to consider.

- (i) If each of v_1 and v_2 is a CV in F_1 and F_2 , respectively, then by Theorem 2.3(i), $\eta(\mathcal{G}) = \eta(G - e) - 1$, and by Theorem 4.4(i), $\eta(\mathcal{G} : e) = \eta(G - e) - 2$. Thus, $\eta(\mathcal{G} : e) = \eta(\mathcal{G}) - 1$.
- (ii) If each of v_1 and v_2 is a CFV_{mid} in F_1 and F_2 , respectively, and by the premise that v is a CV in \mathcal{G} , then by Theorem 2.3(iv), $\eta(\mathcal{G}) = \eta(G - e) + 1$. By Theorem 3.7(iii), the vertices v_1 and v_2 are either both CV or both CFV_{mid} in $\mathcal{G} : e$. In the first case, by Theorem 4.6(ii), $\eta(\mathcal{G} : e) = \eta(G - e) + 1$ and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G})$. In the latter case, by Theorem 4.6(iii), $\eta(\mathcal{G} : e) = \eta(G - e)$ and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G}) - 1$.

■

If what we claim in Remark 5.2 is proved to be true, then $\eta(\mathcal{G} : e)$ can only be equal to $\eta(\mathcal{G}) - 1$ when v is a CV in \mathcal{G} .

Theorem 6.5. *Let \mathcal{G} be a graph with a cut-vertex v . If v is a CFV_{mid} in \mathcal{G} , then $\eta(\mathcal{G} : e)$ is either $\eta(\mathcal{G})$ or $\eta(\mathcal{G}) + 1$.*

Proof. Since v is a CFV_{mid} in \mathcal{G} , then by Theorem 6.2(iii), we have two cases to consider.

- (i) If each of v_1 and v_2 is a CFV_{mid} in F_1 and F_2 , respectively, then since v is a CFV_{mid} in \mathcal{G} , by Theorem 2.3(iv), $\eta(\mathcal{G}) = \eta(G - e)$. By Theorem 3.7(iii), the vertices v_1 and v_2 are again either both CV or both CFV_{mid} in $\mathcal{G} : e$. Thus, either $\eta(\mathcal{G} : e) = \eta(G - e) + 1$ and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G}) + 1$ (by Theorem 4.6(ii)), or $\eta(\mathcal{G} : e) = \eta(G - e)$ and thus $\eta(\mathcal{G} : e) = \eta(\mathcal{G})$ (by Theorem 4.6(iii)).
- (ii) If v_1 is a CV in F_1 and v_2 is a CFV_{mid} in F_2 , then by Theorem 2.3(i), $\eta(\mathcal{G}) = \eta(G - e) - 1$, and by Theorem 4.4(ii), $\eta(\mathcal{G} : e) = \eta(G - e) - 1$. Thus, $\eta(\mathcal{G} : e) = \eta(\mathcal{G})$.

■

Theorems 6.3 to 6.5 yield another inequality of the same type obtained as a consequence of the Interlacing Theorem, this time involving the replacement of a cut-vertex by an edge.

Theorem 6.6. *Let \mathcal{G} be a graph with a cut-vertex v , and let $\mathcal{G} : e$ be the graph \mathcal{G} with the vertex v replaced by the edge e . Then*

$$\eta(\mathcal{G}) - 1 \leq \eta(\mathcal{G} : e) \leq \eta(\mathcal{G}) + 1.$$

References

- [1] D. Ali, J. B. Gauci, I. Sciriha, K. R. Sharaf, Coalescing Fiedler and core vertices, *Czech. Math. J.* (to appear).
- [2] L. Collatz, U. Sinogowitz, Spektren endlicher Grafen, *Abh. Math. Sem. Univ. Hamburg* **21** (1957) 63–77.
- [3] P. W. Fowler, B. T. Pickup, T. Z. Todorova, M. Borg, I. Sciriha, Omni-conducting and omni-insulating molecules, *J. Chem. Phys.* **140** (2014) #054115.
- [4] P. W. Fowler, B. T. Pickup, T. Z. Todorova, R. De Los Reyes, I. Sciriha, Omni-conducting fullerenes, *Chem. Phys. Lett.* **568/569** (2013) 33–35.
- [5] H. H. Günthard, H. Primas, Zusammenhang von Graphentheorie und MO-Theorie von Molekeln mit Systemen konjugierter Bindungen, *Helv. Chim. Acta* **39** (1956) 1645–1653.
- [6] I. Gutman, B. Borovićanin, Nullity of graphs: An updated survey, in: D. Cvetković, I. Gutman (Eds.), *Selected Topics on Applications of Graph Spectra*, Math. Inst., Belgrade, 2011, pp. 137–154.

- [7] E. Heilbronner, Das Kompositions-prinzip: Eine anschauliche Methode zur Elektronen-theore-tischen bechandlung nicht oder neidrig symmetrischer Molekeln im pahmen der MO-Theorie, *Helv. Chim. Acta* **36** (1953) 170–188.
- [8] E. Hückel, Quantentheoretische Beiträge zum Benzolproblem, *Z. Phys.* **70** (1931) 204–286.
- [9] N. B. Ibrahim, On the nullity of some sequential element identified, element introduced graph, *MS thesis*, Univ. Zakho, Duhok, 2013.
- [10] I. J. Kim, B. L. Shader, On Fiedler- and Parter-vertices of acyclic matrices, *Lin. Algebra Appl.* **428** (2008) 2601–2613.
- [11] M. Marcus, H. Minc, *A Survey of Matrix Theory and Matrix Inequalities*, Allyn and Bacon, Boston, 1964.
- [12] B. T. Pickup, P. W. Fowler, M. Borg, I. Sciriha, A new approach to the method of source-sink potentials for molecular conduction, *J. Chem. Phys.* **143** (2015) #194105.
- [13] K. Ruedenberg, Free electron network model for conjugated systems. V. Energies and electron distributions in the F.E.M.O. model and in the L.C.A.O. model, *J. Chem. Phys.* **22** (1954) 1878–1894.
- [14] A. J. Schwenk, Computing the characteristic polynomial of a graph, in: R. A. Bari, F. Harary (Eds.), *Graphs and Combinatorics*, Springer-Verlag, Berlin, 1975, pp. 153–172.
- [15] I. Sciriha, On the construction of graphs of nullity one, *Discr. Math.* **181** (1998) 193–211.
- [16] I. Sciriha, A characterization of singular graphs, *J. Lin. Algebra* **16** (2007) 451–462.
- [17] I. Sciriha, Maximal core size in singular graphs, *Ars Math. Contemp.* **2** (2009) 217–229.
- [18] I. Sciriha, Extremal non-bonding orbitals, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 751–768.
- [19] I. Sciriha, M. Debono, M. Borg, P. W. Fowler, B. T. Pickup, Interlacing-extremal graphs, *Ars Math. Contemp.* **6** (2013) 261–278.
- [20] E. B. Vakhovskii, A technique for the dismantling of a graph, *Siberian Math. J.* **9** (1968) 192–197.