# Nullity of a Graph with a Cut-Edge

Didar A. Ali<sup>1</sup>, John Baptist Gauci<sup>2</sup>, Irene Sciriha\*<sup>2</sup>, Khidir R. Sharaf<sup>1</sup>

<sup>1</sup>Department of Mathematics, Faculty of Science, University of Zakho, Duhok, Iraq Didar.ali@uoz.ac, Khidir.sharaf@uoz.ac

 $^2Department\ of\ Mathematics,\ Faculty\ of\ Science,$   $University\ of\ Malta,\ Msida,\ Malta$ 

john-baptist.gauci@um.edu.mt, irene.sciriha-aquilina@um.edu.mt

(Received March 20, 2016)

#### Abstract

The nullity of a graph is known to be an analytical tool to predict reactivity and conductivity of molecular  $\pi$ -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

<sup>\*</sup>Corresponding author

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  $\lambda_1, \lambda_2, \ldots, \lambda_n$  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  $n \ge 2$  vertices. Then  $\eta(G) - 1 < \eta(G - u) < \eta(G) + 1$ .

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<sub>mid</sub>) if  $\eta(G-u)=\eta(G)$  and an upper core-forbidden vertex (CFV<sub>upp</sub>) if  $\eta(G-u)=\eta(G)+1$ . In the literature, vertices which are CFV<sub>upp</sub> 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  $\pi$ -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<sub>mid</sub>.

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-ebe  $F_1\dot{\cup}F_2$ , where  $F_1-v_1=G_1\dot{\cup}G_2\dot{\cup}\ldots\dot{\cup}G_r$  and  $F_2-v_2=G_{r+1}\dot{\cup}G_{r+2}\dot{\cup}\ldots\dot{\cup}G_s$ , 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  $e = v_1 v_2$ , 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  $e = v_1 v_2$  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  $e = v_1 v_2$  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).

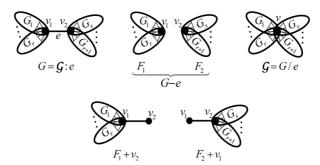


Figure 1. The graphs  $G = \mathcal{G} : e, G - e = F_1 \dot{\cup} F_2, \mathcal{G} = G/e, F_1 + v_2 \text{ and } F_2 + v_1,$  where  $e = v_1 v_2$ .

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<sub>upp</sub> 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<sub>upp</sub>.

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<sub>upp</sub> 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<sub>upp</sub> in  $H_1$  and  $v_2$  is a CFV<sub>mid</sub> in  $H_2$ , then  $\eta(H) = \eta(H_1) + \eta(H_2)$ .
- (iii) If each of  $v_1$  and  $v_2$  is a CFV<sub>upp</sub> 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<sub>mid</sub> in the respective component graph, then either v is a CFV<sub>mid</sub> 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<sub>upp</sub> in  $F_1 + v_2$ .

Proof. Since each vertex of  $K_2$  is a CFV<sub>upp</sub> 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<sub>upp</sub> in  $F_1+v_2$ .

Conversely, let  $v_2$  be a CFV<sub>upp</sub> 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<sub>mid</sub> 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<sub>mid</sub> in  $F_1$  if and only if  $v_2$  is a CFV<sub>mid</sub> in  $F_1 + v_2$ .

*Proof.* If  $v_1$  is a CFV<sub>mid</sub> 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<sub>mid</sub> in  $F_1 + v_2$ .

Conversely, let  $v_2$  be a CFV<sub>mid</sub> 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<sub>mid</sub> in  $F_1$ .

The case when  $v_1$  is a CFV<sub>upp</sub> 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<sub>upp</sub> 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<sub>mid</sub> 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  $\lambda$  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

$$\phi(G) = \phi(F_1 + v_2)\phi(F_2 - v_2) + \phi(F_1)\phi(F_2) - \lambda\phi(F_1)\phi(F_2 - v_2)$$

$$= (\lambda\phi(F_1) - \phi(F_1 - v_1))\phi(F_2 - v_2) + \phi(F_1)\phi(F_2) - \lambda\phi(F_1)\phi(F_2 - v_2)$$

$$= \phi(F_1)\phi(F_2) - \phi(F_1 - v_1)\phi(F_2 - v_2)$$

$$= \phi(G - e) - \phi(G - \{v_1, v_2\}).$$

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<sub>upp</sub> in  $H_1$  or  $v_2$  is a CFV<sub>upp</sub> in  $H_2$ , then v is a CFV<sub>upp</sub> in H.
- (ii) If each of v<sub>1</sub> and v<sub>2</sub> 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<sub>1</sub> and v<sub>2</sub> is a CFV<sub>mid</sub> in the respective component graph, then v is either a CFV<sub>mid</sub> 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<sub>mid</sub> in  $F_2 + v_1$ , or if  $v_1$  is a CFV<sub>mid</sub> in  $F_1$  and a CV in  $F_2 + v_1$ , then  $v_1$  is a CFV<sub>mid</sub> in G.
- (iv) If  $v_1$  is a CFV<sub>mid</sub> in each of  $F_1$  and  $F_2 + v_1$ , then  $v_1$  is either a CFV<sub>mid</sub> 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<sub>upp</sub> 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<sub>mid</sub> 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<sub>mid</sub> in  $F_2$ , then  $v_1$  is a CFV<sub>mid</sub> and  $v_2$  is a CFV<sub>upp</sub> in G.

*Proof.* Since  $v_1$  is a CV in  $F_1$ , then by Theorem 3.4,  $v_2$  is a CFV<sub>upp</sub> in G. By Theorem 2.5, since  $v_2$  is a CFV<sub>mid</sub> in  $F_2$ , then  $v_1$  is also a CFV<sub>mid</sub> in  $F_2 + v_1$ . Thus, by Theorem 3.3(iii),  $v_1$  is a CFV<sub>mid</sub> in G.

If we know that at least one of the root vertices of  $F_1$  and  $F_2$  is a CFV<sub>upp</sub>, 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<sub>upp</sub> 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<sub>upp</sub> in  $F_1$ , by Theorem 3.3(i),  $v_1$  is a CFV<sub>upp</sub> 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<sub>upp</sub> in  $F_2$ , then by Theorem 3.2(i),  $v_2$  is a CFV<sub>upp</sub> 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<sub>mid</sub> in  $F_2$ , then by Theorem 3.2(iii),  $v_2$  is a CFV<sub>mid</sub> 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<sub>1</sub> and v<sub>2</sub> is a CV in F<sub>1</sub> and F<sub>2</sub>, respectively, then each of v<sub>1</sub> and v<sub>2</sub> is a CFV<sub>upp</sub> in G.
- (ii) If each of v<sub>1</sub> and v<sub>2</sub> is a CFV<sub>upp</sub> in F<sub>1</sub> and F<sub>2</sub>, respectively, then each of v<sub>1</sub> and v<sub>2</sub> is a CFV<sub>upp</sub> in G.
- (iii) If each of  $v_1$  and  $v_2$  is a CFV<sub>mid</sub> in  $F_1$  and  $F_2$ , respectively, then  $v_1$  and  $v_2$  are either both CV or both CFV<sub>mid</sub> 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<sub>mid</sub> 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<sub>mid</sub> 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<sub>upp</sub> 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<sub>mid</sub> 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
$CFV_{upp}$	$\mathrm{CFV}_{\mathrm{mid}}$	$CFV_{upp}$	$CFV_{mid}$
CV	CV	$CFV_{upp}$	$CFV_{upp}$
CV	$CFV_{mid}$	$CFV_{mid}$	$CFV_{upp}$
$\mathrm{CFV}_{\mathrm{mid}}$	$\mathrm{CFV}_{\mathrm{mid}}$	$CFV_{mid}$	$CFV_{mid}$
		CV	CV

**Table 2.** Type of the vertices incident to a cut-edge  $e = v_1 v_2$ .

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<sub>mid</sub> 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<sub>mid</sub> in  $F_1$  and  $F_2$ , respectively;
- (ii) v<sub>1</sub> and v<sub>2</sub> correspond to non-zero entries on exactly one kernel eigenvector in a basis for the nullspace of A(G).

Proof. From Table 2,  $v_1$  and  $v_2$  are both CV in G if they are both CFV<sub>mid</sub> 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  $\mathbf{x}^{(i)}_{\text{res.}}$  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  $\mathbf{x}^{(i)}_{\text{res.}}$  is a kernel eigenvector of  $\mathbf{A}(G-v_1)$ . Since  $\eta(G-v_1) = \eta - 1$ , then  $\mathbf{x}^{(1)}_{\text{res.}}, \mathbf{x}^{(2)}_{\text{res.}}, \dots, \mathbf{x}^{(\eta-1)}_{\text{res.}}$  are  $\eta - 1$  linearly independent eigenvectors generating the nullspace of  $\mathbf{A}(G-v_1)$ . Suppose there is some  $\mathbf{x}^{(i)}_{\text{res.}}$ , 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  $e \in E(G)$ ,  $|\eta(G) - \eta(G - e)| \le 2$ .

*Proof.* Let  $e = v_1 v_2$ . By Theorem 1.2,  $\eta(G) - 1 \le \eta(G - v_1) \le \eta(G) + 1$ . 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  $\eta(G) - 2 \le \eta(G - v_1 + v') \le \eta(G) + 2$ . 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	$\Diamond$	1	$\Diamond \Diamond \Diamond$	3
	$\Diamond$	2	$\Diamond \Diamond$	4
-1	$\Diamond$	1		2
	$\triangleright$	1	$\triangleright \diamondsuit$	2
0	$\rightarrow$	1	$\overline{}$	1
	$\triangleright \!$	1	$\triangleright \Leftrightarrow$	1
1		2		1
		2		1
2	$\Diamond \Diamond \Diamond$	3	$\langle \vee \rangle$	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<sub>upp</sub> 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<sub>upp</sub> 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<sub>upp</sub> 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<sub>upp</sub>, 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<sub>upp</sub> 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<sub>mid</sub> 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<sub>upp</sub> 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<sub>upp</sub> in  $F_2 + v_1$  and a CFV<sub>mid</sub> in  $F_1$ , or if  $v_1$  is a CFV<sub>mid</sub> in  $F_2 + v_1$  and a CFV<sub>upp</sub> in  $F_1$ , then  $\eta(G) = \eta(G e) 1$ .

*Proof.* By Theorem 2.4, the vertex  $v_1$  is a CFV<sub>upp</sub> in  $F_2 + v_1$  if and only if  $v_2$  is a CV in  $F_2$ , and  $v_2$  is a CFV<sub>upp</sub> 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<sub>mid</sub> 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<sub>mid</sub> in  $F_1$  and a CFV<sub>upp</sub> in G, then  $\eta(G) = \eta(G e) 1$ .
- (ii) If  $v_1$  is a CFV<sub>mid</sub> in  $F_1$  and a CV in G, then  $\eta(G) = \eta(G-e) + 1$ .
- (iii) If  $v_1$  is a CFV<sub>mid</sub> in  $F_1$  and a CFV<sub>mid</sub> in G, then  $\eta(G) = \eta(G e)$ . Proof.
  - (i) Since  $v_1$  is a CFV<sub>upp</sub> 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<sub>mid</sub> 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<sub>mid</sub> 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<sub>mid</sub> in  $F_1$ , implying that  $\eta(G v_1) = \eta(F_1) + \eta(F_2) = \eta(G e)$ . Since  $v_1$  is a CFV<sub>mid</sub> 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  $\eta(G) - 1 \le \eta(G - e) \le \eta(G) + 2$ .

*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<sub>upp</sub> in  $F_1$  or  $v_2$  is a CFV<sub>upp</sub> 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<sub>mid</sub> in  $F_2$ , or  $v_1$  is a CFV<sub>mid</sub> 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<sub>1</sub> and v<sub>2</sub> is a CFV<sub>mid</sub> in F<sub>1</sub> and F<sub>2</sub>, respectively, then by Theorem 3.7(iii), v<sub>1</sub> and v<sub>2</sub> are either both CV or both CFV<sub>mid</sub> in G. If they are both CV in G, then by Theorem 4.6(ii), η(G) = η(G e) + 1; whilst if they are both CFV<sub>mid</sub> in G, then by Theorem 4.6(iii), η(G) = η(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<sub>upp</sub> in G, then v is either a CFV<sub>upp</sub> or a CV in G/e and  $\eta(G/e) = \eta(G) + 1$ .
- (ii) If  $v_1$  is a CFV<sub>upp</sub> in G and  $v_2$  is a CV in G, then v is a CFV<sub>upp</sub> in G/e and  $\eta(G/e) = \eta(G) 1$ .
- (iii) If  $v_1$  is a CFV<sub>upp</sub> in G and  $v_2$  is a CFV<sub>mid</sub> in G, then v is either a CFV<sub>upp</sub> or a CFV<sub>mid</sub> in G/e and  $\eta(G/e) = \eta(G)$ .
- (iv) If  $v_1$  and  $v_2$  are both CFV<sub>mid</sub> in G, then either v is a CFV<sub>mid</sub> 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<sub>mid</sub> 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<sub>mid</sub> 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<sub>upp</sub> 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  $F_1 - v_1 = \{G_1, \ldots, G_r\}$  and  $F_2 - v_2 = \{G_{r+1}, \ldots, G_s\}$  for some  $r \in \{1, \ldots, s-1\}$ . The graph  $\mathcal{G} : e$  is constructed by introducing the edge  $e = v_1v_2$  in  $F_1\dot{\cup}F_2$ . Note that  $\mathcal{G} : e$  is identical to the graph  $\mathcal{G}$  with cut-edge  $v_1v_2$ .

The following theorem follows immediately from Theorem 5.1.

**Theorem 6.1.** Let v be a cut-vertex in  $\mathcal{G}$  and let  $e = v_1v_2$  in  $\mathcal{G}$ : e.

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

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<sub>mid</sub> in  $H_1$  and  $H_2$ .
- (ii) The vertex v is a CFV<sub>upp</sub> in G if and only if at least one of v<sub>1</sub> and v<sub>2</sub> is a CFV<sub>upp</sub> in H<sub>1</sub> or H<sub>2</sub>.
- (iii) If v is a CFV<sub>mid</sub> in G, then either v<sub>1</sub> and v<sub>2</sub> are both CFV<sub>mid</sub> in H<sub>1</sub> and H<sub>2</sub>, or v<sub>1</sub> is a CFV<sub>mid</sub> in H<sub>1</sub> and v<sub>2</sub> is a CV in H<sub>2</sub>.

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

*Proof.* Since v is a CFV<sub>upp</sub> in  $\mathcal{G}$ , by Theorem 6.2(ii), either  $v_1$  is a CFV<sub>upp</sub> in  $F_1$  or  $v_2$  is a CFV<sub>upp</sub> 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<sub>upp</sub> 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<sub>upp</sub> in  $F_1$  and  $v_2$  is a CFV<sub>mid</sub> 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<sub>upp</sub> 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<sub>mid</sub> 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<sub>mid</sub> 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<sub>mid</sub> in  $\mathcal{G}$ , then  $\eta(\mathcal{G}:e)$  is either  $\eta(\mathcal{G})$  or  $\eta(\mathcal{G})+1$ .

*Proof.* Since v is a CFV<sub>mid</sub> 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<sub>mid</sub> in  $F_1$  and  $F_2$ , respectively, then since v is a CFV<sub>mid</sub> 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<sub>mid</sub> 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<sub>mid</sub> 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

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

#### 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, Omniconducting 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 dismounting of a graph, Siberian Math. J. 9 (1968) 192–197.