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Connected sum of graphs as molecular electronic devices

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Abstract

The connected sum Z of two root graphs of order n is obtained by gluing them together along a common subgraph G of order $n-1$. The two vertices of Z not in G are called terminal vertices. The edged connected sum $Z+e$ is obtained from Z by adding the edge joining the terminal vertices. We consider the case when the root graphs have the same μ–eigenspace of the 0–1 adjacency matrix of dimension one. We show that the μ–eigenspace imposes structural constraints on Z and $Z+e$, depending on the type of the two vertices. For $\mu = 0$, we investigate the electrical behaviour of a molecular electronic device with structure Z or $Z+e$, connected at the terminal vertices in a circuit across a small bias voltage. It transpires that the device will be a conductor or insulator depending on the type of the terminal vertices in the 0–eigenspace. We show that conductivity or its barring distinguishes between Z and $Z+e$.

Keywords: Molecular electronic device (MED), common eigenspace, μ–core vertices, connected–sum.

Math. Subj. Class.: 05C60, 05C07, 05C50, 15A18, 05B20 (chemistry).

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1 Preliminaries

A graph $G(\mathcal{V},\mathcal{E})$ of order n has a non–empty vertex set $\mathcal{V} = \{1,\dots,n\}$ and an edge set $\mathcal{E}$ consisting of couples of vertices. The subgraph $G-v$ is obtained from G by deleting the vertex v. We write $G-z_1-z_2$ for the graph obtained from G by deleting two distinct vertices z_1 and z_2 in $\mathcal{V}$.

The graphs we consider are simple, that is, they have no multiple edges or loops. The 0–1 *adjacency matrix* $\mathbf{G} = (a_{ij})$ of a labelled graph G on n vertices is the $n \times n$ matrix such that $a_{ij} = 1$ if there is an edge between the vertices i and j, and $a_{ij} = 0$ otherwise. The *spectrum* of G consists of the *eigenvalues of* G, which are those of the matrix $\mathbf{G}$. A

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graph with two distinguished vertices z_1 and z_2 is called a *device* with terminal vertices z_1 and z_2.

We write $G_1 \equiv G_2$ for two isomorphic graphs with the same vertex labels. The proof of the main result uses the connected–sum of two graphs, a concept analogous to the operation by the same name in topology. The connected–sum of two labelled graphs is obtained by gluing them together at a common subgraph. If in the two graphs H_1 and H_2, $H_1 - z_1 \equiv H_2 - z_2 \equiv G$, then the connected-sum Z of H_1 and H_2 is formed from their disjoint union by identifying pairs of same labelled vertices of G, in these two subgraphs, to form a single shared subgraph. In Z, the vertices z_1 and z_2 are non–adjacent. On adding the edge $\{z_1, z_2\}$, the *edged connected–sum* $Z + e$, is obtained.

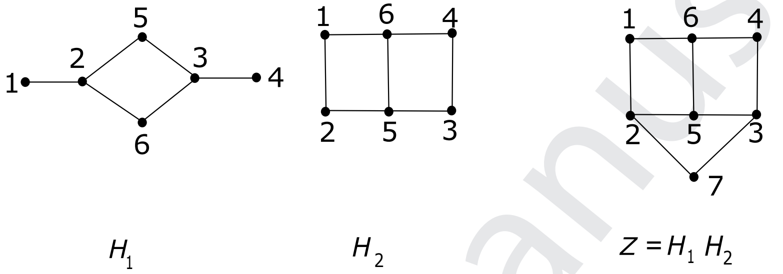

Figure 1: Connected–sum of H_1 and H_2 having a common subgraph $H_i - 6$.

Figure 1 shows a pair of non–isomorphic graphs H_1 and H_2. The path $P_5 \equiv H_1 - 6 \equiv H_2 - 6$. Their connected–sum Z is obtained from P_5 by adding the two vertices labelled 6 and 7 adjacent to the same neighbours as those of vertex 6 in H_1 and vertex 6 in H_2.

In the sequel, we shall form the connected–sum of two connected n–vertex graphs $\mathcal{H}_1$ and $\mathcal{H}_2$, of order $n \geq 3$, sharing a common simple eigenvalue μ with an eigenspace generated by the same vector $\mathbf{x}$. The multiplicity η_μ of the eigenvalue μ of their adjacency matrix is therefore equal to one. The graphs $\mathcal{H}_1$ and $\mathcal{H}_2$, are chosen such that for some vertex z_1 in $\mathcal{H}_1$ and some vertex z_2 in $\mathcal{H}_2$, $\mathcal{H}_1 - z_1 \equiv \mathcal{H}_2 - z_2 \equiv G$. The graphs $\mathcal{H}_1$ and $\mathcal{H}_2$, satisfying these conditions, are termed *root–graphs* of Z or $Z + e$. It follows immediately that the label of z_1 in $\mathcal{H}_1$ is the same as that of z_2 in $\mathcal{H}_2$. Unless otherwise specified, the labels of the vertices z_1 and z_2 are the last in the two graphs $\mathcal{H}_1$ and $\mathcal{H}_2$.

A singular graph has the eigenvalue 0. Singular configurations necessarily occur in singular graphs [10]. They are graphs on the least number of vertices for specific non–zero entries in a vector spanning the nullspace of their adjacency matrix. A list of the singular configurations for up to five non zero entries is found in [8] and selected larger ones are given in [9]. When searching for all feasible singular configurations, it was observed that for a particular eigenvector, certain pairs of singular configurations share an identical vertex–deleted subgraph. This motivated the concept of the connected–sum of two graphs, which are its induced subgraphs. The connected–sum turns out to have surprising structural and spectral properties. We shall see in Section 6, that the connected sum and the edged connected sum are of different types (insulator or conductor) if the terminals are core vertices in their respective graphs.

2 Vertex types in root graphs

The well known *Cauchy's Interlacing Theorem* on the distribution of the eigenvalues of a real symmetric matrix permits the multiplicity η_μ of an eigenvalue μ, in the spectrum of a graph, to change by at most one on the deletion or addition of a vertex u from or to a graph, respectively. Therefore $\eta_\mu(G) - 1 \leq \eta_\mu(G-u) \leq \eta_\mu(G) + 1$ [6, p.119].

A vertex u in a graph G can be one of three *types*, depending on the difference of $\eta_\mu(G-u)$ from $\eta_\mu(G)$. Following the terminology used in [1, 4, 11, 12], a vertex u is a core vertex (μ–cv), a *middle μ–core–forbidden vertex* (μ–cfv$_{\text{mid}}$) or an *upper core–forbidden vertex* (μ–cfv$_{\text{upp}}$) if the nullity of the graph $G-u$ obtained from G upon deleting the vertex u is $\eta_\mu(G) - 1$, $\eta_\mu(G)$ or $\eta_\mu(G) + 1$, respectively. Note that the kth entry of all μ–eigenvectors is zero if and only if removal of vertex k does not cause a reduction in the number of linearly independent μ–eigenvectors of $G - k$, which is therefore $\eta_\mu(G)$ or $\eta_\mu(G) + 1$. The next result follows immediately.

Proposition 2.1. *The multiplicity of an eigenvalue μ reduces by one on deletion of a vertex u from a graph G if and only if u is a μ–cv of G.*

First we determine a result on the type of vertices z_1 and z_2 in the connected–sum of the graphs Z. In the sequel the graph G will be equivalent to $\mathcal{H}_1 - z_1$ and $\mathcal{H}_2 - z_2$.

Lemma 2.2. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$, be root graphs. Then,*

(i) *in $\mathcal{H}_1$ and $\mathcal{H}_2$, the two vertices z_1 and z_2 are of the same type;*

(ii) *in Z and $Z + e$, the two vertices z_1 and z_2 are of the same type (not necessarily the same in the different graphs Z and $Z + e$).*

Proof. Recall that $\mathcal{H}_1$ and $\mathcal{H}_2$ have a one dimensional μ–eigenspace and share the same vertex–deleted subgraph $G \equiv \mathcal{H}_1 - z_1 \equiv \mathcal{H}_2 - z_2$. Hence the change in the multiplicity of μ from the common one of the root graphs to that of G is the same. This proves (i).

To prove (ii), suppose, for contradiction, that z_1 and z_2 are not of the same type in Z. Then, deleting z_1 from Z, (or $Z + e$,) yields the graph $\mathcal{H}_2$, which has a different dimension of the μ–eigenspace to that of $\mathcal{H}_1$, obtained on deleting z_2 from Z, (or $Z + e$,). This contradicts the definition of $\mathcal{H}_1$ and $\mathcal{H}_2$, which states that $\eta_\mu(\mathcal{H}_1) = \eta_\mu(\mathcal{H}_2) = 1$. □

3 The structure of the connected–sum

In this section, we show that the connected sum has a structure depending on the vertex type of z_1 and z_2 in the root graphs.

Twin vertices may be duplicate or co–duplicate. *Duplicate vertices* are non–adjacent and have the same open neighbourhood in a graph. *Co–duplicate vertices* are adjacent and have the same closed neighbourhood in a graph. If they are the last labelled vertices in a graph, then $(\mathbf{0}, 1, -1)^t$ is an eigenvector of the 0–1–adjacency matrix, with associated eigenvalue 0 for duplicate vertices and -1 for co–duplicate vertices.

3.1 μ–cv terminal vertices

When z_1 and z_2 are μ–cv, the last entry of a common μ–eigenvector $\mathbf{x}$ of $\mathcal{H}_1$ and of $\mathcal{H}_2$ is non–zero, that is, there exist $\mathbf{v} \neq \mathbf{0}$ and $\alpha \neq 0$ such that $\mathbf{x} = \begin{pmatrix} \mathbf{v} \\ \hline \alpha \end{pmatrix}$. Note that for a connected graph (and in particular for no isolated vertices), $\mathbf{x}$ contains at least two non–zero entries.

Remark 3.1. Let $\mathbf{G}$ be the adjacency matrix of the graph $G \equiv \mathcal{H}_1 - z_1 \equiv \mathcal{H}_2 - z_2$ and $\mathbf{F} = \mathbf{G} - \mu\mathbf{I}$. Since for $i \in \{1, 2\}$, $\eta_\mu(\mathcal{H}_i) = 1$, $\mathbf{Fv} \neq 0$. Letting $\mathbf{z_1}$ and $\mathbf{z_2}$ denote the characteristic vectors representing the adjacencies of z_1 and z_2 to the vertices of G, we obtain

$$(\mathbf{H_1} - \mu\mathbf{I})\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\end{array}\right) = \left(\begin{array}{c|c}\mathbf{F} & \mathbf{z_1}\\ \hline {\mathbf{z_1}}^t & -\mu\end{array}\right)\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\end{array}\right) = \left(\begin{array}{c}\mathbf{Fv} + \alpha\mathbf{z_1}\\ \hline {\mathbf{z_1}}^t\mathbf{v} - \mu\alpha\end{array}\right) = \mathbf{0} \tag{3.1}$$

and

$$(\mathbf{H_2} - \mu\mathbf{I})\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\end{array}\right) = \left(\begin{array}{c|c}\mathbf{F} & \mathbf{z_2}\\ \hline {\mathbf{z_2}}^t & -\mu\end{array}\right)\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\end{array}\right) = \left(\begin{array}{c}\mathbf{Fv} + \alpha\mathbf{z_2}\\ \hline {\mathbf{z_2}}^t\mathbf{v} - \mu\alpha\end{array}\right) = \mathbf{0}, \tag{3.2}$$

for some $\mathbf{v} \neq \mathbf{0}$ and $\alpha \neq 0$.

We now seek to lift (if possible) the common μ–eigenvector of $\mathcal{H}_1$ and $\mathcal{H}_2$ to the μ–eigenspace of the connected–sum Z in which z_1 and z_2 are non–adjacent and for the edged $Z + e$, where e is the edge $\{z_1, z_2\}$.

Theorem 3.2. *If z_1 and z_2 are μ–cv in $\mathcal{H}_1$ and in $\mathcal{H}_2$, respectively, then they are duplicate vertices in Z and co-duplicate vertices in $Z + e$.*

Proof. Using the notation in Remark 3.1 above, let $\mathbf{Y}$ denote the adjacency matrix of Z or $Z + e$. In the last two columns, vectors $\mathbf{z_1}$ and $\mathbf{z_2}$ are again the characteristic vectors representing the adjacencies of z_1 and z_2 to the vertices of G. Writing $\mathbf{F} = \mathbf{G} - \mu\mathbf{I}$, since $\mathbf{Fv} \neq 0$,

$$(\mathbf{Y} - \mu\mathbf{I})\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\\ \alpha\end{array}\right) = \left(\begin{array}{c|cc}\mathbf{F} & \mathbf{z_1} & \mathbf{z_2}\\ \hline {\mathbf{z_1}}^t & -\mu & a\\ {\mathbf{z_2}}^t & a & -\mu\end{array}\right)\left(\begin{array}{c}\mathbf{v}\\ \hline \alpha\\ \alpha\end{array}\right) = \left(\begin{array}{c}\mathbf{Fv} + \alpha\mathbf{z_1} + \alpha\mathbf{z_2}\\ \hline {\mathbf{z_1}}^t\mathbf{v} - \alpha\mu + \alpha a\\ {\mathbf{z_2}}^t\mathbf{v} - \alpha\mu + \alpha a\end{array}\right) \tag{3.3}$$

$$= \left(\begin{array}{c}\alpha\mathbf{z_2}\\ \hline \alpha a\\ \alpha a\end{array}\right) = \left(\begin{array}{c}\alpha\mathbf{z_1}\\ \hline \alpha a\\ \alpha a\end{array}\right), \quad \text{for } \alpha \neq 0, \text{ using (3.1) and (3.2),}$$

where a is 1 in $Z + e$ and 0 in Z. Hence $\mathbf{z}_1 = \mathbf{z}_2$. ☐

Note that for $\mu \neq 0$, $\eta_\mu(Z) = 0$ and for $\mu \neq -1$, $\eta_\mu(Z + e) = 0$.

If z_1 and z_2 are 0–cv in $\mathcal{H}_1$ and in $\mathcal{H}_2$, respectively, then $\eta_0(Z) = 2$. Similarly, If z_1 and z_2 are (-1)–cv in $\mathcal{H}_1$ and in $\mathcal{H}_2$, respectively, then $\eta_{-1}(Z + e) = 2$.

Corollary 3.3. *If z_1 and z_2 are μ–cv in the root graphs $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $\mathcal{H}_1 \equiv \mathcal{H}_2$.*

We have shown that a device Y, which is a connected sum with terminal vertices that are μ–cv in the root graphs, has particular structural properties. The terminal vertices in Y must be duplicate vertices. Figure 2 shows the root graphs isomorphic to C_6, Z with duplicate vertices and $Z + e$ with a co–duplicate vertices. For the eigenvalue 2, any vertex of C_6 is a 2–cv. None of the graphs Z or $Z + e$ has the eigenvalue 2.

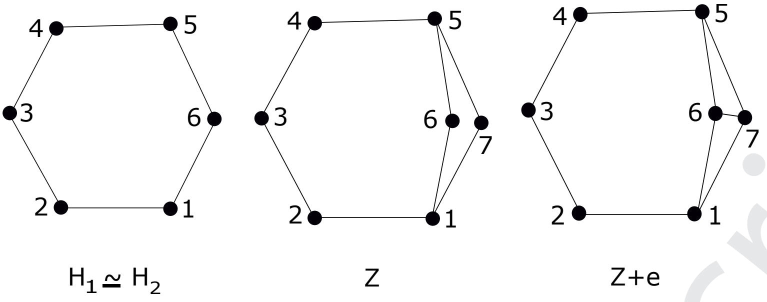

Figure 2: 2–cv in root graphs C_6.

4 μ–core–forbidden vertices in the root–graphs

When z_1 and z_2 are μ–cfv, the last entry of a common μ–eigenvector $\mathbf{x}$ of $\mathcal{H}_1$ and of $\mathcal{H}_2$ is zero.

Lemma 4.1. *Let z_1 and z_2 be μ–cfv in the root graphs $\mathcal{H}_1$ and $\mathcal{H}_2$ which form the connected sum Z. Then μ is an eigenvalue of both Z and $Z + e$ with multiplicity 1 or 2.*

Proof. There exists $\mathbf{v} \neq \mathbf{0}$ such that $\mathbf{x} = \begin{pmatrix} \mathbf{v} \\ \hline 0 \end{pmatrix}$ is a μ eigenvector of each root graph that can be lifted to the μ eigenvector $(\mathbf{x}, 0)^t = (\mathbf{v}, 0, 0)^t$ of both Z and $Z + e$.

Since the dimension of the μ–eigenspace of the root graphs is 1, by interlacing, the μ–multiplicity of Z and $Z + e$ is 1 or 2. □

Adopting the notation used in Remark 3.1, $\mathbf{F} = \mathbf{G} - \mu\mathbf{I}$. Let W is the adjacency matrix of Z or $Z + e$.

Therefore,

$$(\mathbf{H_i} - \mu\mathbf{I})\mathbf{x} = (\mathbf{H_i} - \mu\mathbf{I}) \begin{pmatrix} \mathbf{v} \\ \hline 0 \end{pmatrix} = \left(\begin{array}{c|c} \mathbf{F} & \mathbf{z_i} \\ \hline \mathbf{z_i}^t & -\mu \end{array}\right) \begin{pmatrix} \mathbf{v} \\ \hline 0 \end{pmatrix} = \begin{pmatrix} \mathbf{F}\mathbf{v} \\ \hline \mathbf{z_i}^t\mathbf{v} \end{pmatrix} = \mathbf{0}$$

and

$$(\mathbf{W} - \mu\mathbf{I}) \begin{pmatrix} \mathbf{v} \\ \hline 0 \\ 0 \end{pmatrix} = \left(\begin{array}{c|cc} \mathbf{F} & \mathbf{z_1} & \mathbf{z_2} \\ \hline \mathbf{z_1}^t & -\mu & \alpha \\ \mathbf{z_2}^t & \alpha & -\mu \end{array}\right) \begin{pmatrix} \mathbf{v} \\ \hline 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{F}\mathbf{v} \\ \hline \mathbf{z_1}^t\mathbf{v} \\ \mathbf{z_2}^t\mathbf{v} \end{pmatrix}.$$

The following result points to another structural property. Connected sum with core–forbidden vertices in the root–graphs excludes a class of graphs determined by a multiplicity signature (to be defined in Section 5).

Theorem 4.2. *The multiplicity of μ in Z (or $Z + e$) is 2 if and only if z_1 and z_2 correspond to non–zero entries in exactly one μ–eigenvector of some basis of the μ–eigenspace for the graph Z (or $Z + e$).*

Proof. Since each of the root graphs has a one–dimensional μ–eigenspace, the multiplicity of μ in Z (or $Z + e$) is 2 if and only if each of the vertices z_1 and z_1 is a core vertex in Z (or $Z + e$). From Lemma 4.1, a necessary and sufficient condition is that there is a μ–eigenvector, linearly independent of $(\mathbf{x}, 0)^t = (\mathbf{v}, 0, 0)^t$, with non–zero entries at positions z_1 and z_1. This means that there exists a basis for the μ–eigenspace with exactly one eigenvector having non–zero entries at positions z_1 and z_1. □

5 Structure of μ–eigenspace

Theorems 3.2 and 4.2 suggest that the μ–eigenspace imposes graph structure on Z and $Z+e$ beyond that forced by the definition of connected sum. By Lemma 2.2, a connected sum cannot have terminal vertices of different types. The structure of Z and $Z + e$ depends on the common type of the terminal vertices z_1 and z_2. For a device Y, which is a connected sum with terminal vertices that are μ–cv in the root graphs, only duplicate terminal vertices are allowed in Y. We shall now interpret the structure of a device, implied by Theorem 4.2, which is a connected sum with terminal vertices that are μ–cfv in the root graphs. We present some new notation.

Definition 5.1. Let z_1 and z_2 be two vertices of a connected graph W. The *multiplicity signature* $(\eta, \eta_{z_1}, \eta_{z_2}, \eta_{z_1 z_2})$ of W is the sequence of the μ–multiplicities of four graphs: η of W, η_{z_1} of $W - z_1$, η_{z_2} of $W - z_2$ and $\eta_{z_1 z_2}$ of $W - z_1 - z_2$.

Recall that Cauchy's interlacing theorem for a fixed η allows a change of eigenvalue multiplicity of at most one when a vertex is deleted. Therefore, the number of potential multiplicity signatures for a fixed η is 45. There are, however, further restrictions imposed by Jacobi's identity $j^2 = ut - sv$ relating the ℓkth entry j of the adjugate $adj((\lambda - \mu)\mathbf{I} - \mathbf{W})$ of $(\lambda - \mu)\mathbf{I} - \mathbf{W}$ with the four characteristic polynomials s, u, t and v of W, $W - z_1$, $W - z_2$ and $W - z_1 - z_2$, respectively, namely $\phi(W, \lambda - \mu)$, $\phi(W - z_1, \lambda - \mu)$, $\phi(W - z_2, \lambda - \mu)$ and $\phi(W - z_1 - z_2, \lambda - \mu)$, respectively.

Jacobi's identity forces the polynomial $ut - sv$ in λ to have an even number of roots equal to μ, thus ruling out certain multiplicity signatures. Out of the 45 potential multiplicity signatures, only 11 are possible, giving rise to a classification of all graphs with μ–multiplicity η into 11 classes [14, Chapter 7]. This is best possible as graphs were found in each of the 11 classes [2, 5, 7].

A μ–eigenvector of a connected graph contains at least two non–zero entries. As seen in [14] and [3, Chapter 3], for an η–dimensional μ–eigenspace of the adjacency matrix of a connected graph X, Hall's Marriage problem for sets, or the Rado–Hall Theorem for matroids, guarantees a vertex–subset S of η distinct vertex–representatives of the vectors in a basis B_X for the η–dimensional μ–eigenspace [13]. Deleting a vertex representative u in S produces the subgraph $X - u$ having $\eta - 1$ linearly independent μ–eigenvectors associated with the vertex representatives in $S \backslash u$, restricted to $X - u$. Thus, on deletion of u, the μ–eigenvector in B_X associated with u is destroyed and the non–zero entries of the other $\eta - 1$ μ–eigenvectors in B_X are preserved in the μ–eigenspace of $X - u$.

One feasible μ–multiplicity signature is $(\eta, \eta - 1, \eta - 1, \eta - 2)$. If all pairs of distinct vertices of a graph W have this nullity signature, then W is a *uniform μ–core–graph* [13]. The dimension of its μ–eigenspace is at least two.

There exists a basis for the μ–eigenspace of a uniform μ–core–graph consisting of vectors, none of which has two non-zero entries associated with vertices in S in one eigenvector alone. Thus, in a uniform μ–core–graph, any two vertices in S have corresponding non-zero entries in at least two μ–eigenvectors.

Theorem 5.2. *A device* (W, z_1, z_2) *which has* μ–cfv z_1 *and* z_2 *in the root graphs cannot be a uniform* μ*–core–graph.*

Proof. From Theorem 4.2, a basis for the 2-dimensional μ–eigenspace of the device W exists with one μ–eigenvector, linearly independent of $(\mathbf{x}, 0)^t = (\mathbf{v}, 0, 0)^t$, having non–zero entries at positions z_1 and z_1. Thus one of the axioms of a uniform μ–core graph is violated. $\square$

It is worth mentioning that for $\mu = 0$, a uniform μ–core graph X is an omni–insulator in the sense that no electricity flows through the carbon molecule with associated molecular graph X, for any pair of terminal vertices.

6 Molecular electronic devices

In this section the eigenvalue μ is taken to be 0. A device (X, z_1, z_2) is a molecular electronic device (MED) if X is the graph of the molecular structure of a Π–system. The vertices of X represent the carbon atoms of the molecule and the edges are the π bonds that exist between some pairs of carbon atoms. The carbon skeleton of a conjugated carbon molecule has vertex degree at most 3, but here the theory extends to molecular graphs of any degree. In a 3-regular graph, for instance, each carbon atom contributes an electron to the pool of delocalized electrons of the neutral molecule, to produce a Π–system. If the connected sum is the the molecular graph considered, we shall see that only certain multiplicity signatures are possible.

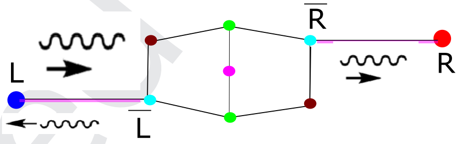

Figure 3: Device with terminal vertices $\tilde{L}$ and $\tilde{R}$ and two semi–infinite wires $L\tilde{L}$ and $R\tilde{R}$.

Ernzerhof's source-and-sink-potential (SSP) model for ballistic conduction in conjugated Π–systems predicts transmission of electrons through a two-wire device in terms of characteristic polynomials of the molecular graph and certain of its subgraphs based on the types of the terminal vertex connections in X. In the graph-theoretical tight–binding version, a device is represented as a molecular graph X attached by internal vertices (atoms) $\tilde{L}$ and $\tilde{R}$ to source (L) and sink (R) vertices, as shown in Figure 3. In steady-state ballistic conduction, a fraction of an incoming electron is reflected back and the rest transmitted through two semi-infinite wires $L\bar{L}$ and $R\bar{R}$.

The Fermi level of Π–electron energy is approximately zero and lies between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital

(LUMO). It is the energy at which the probability of occupying an electronic state is 0.5. The electron transmission $T(0)$ through a conjugated hydrocarbon across which there is a small bias voltage is

$$T(0) = \lim_{E \to 0} T(E) = \lim_{E \to 0} \frac{4\jmath^2 \tilde{\beta}^2}{[(s - v\tilde{\beta}^2)^2 + (u+t)^2 \tilde{\beta}^2]},$$

where $\tilde{\beta}$ is a device parameter and the Jacobi–Sylvester relation $\jmath^2 = ut - sv$ expresses $\jmath$ in terms of u, t, s and v which are all functions of E.

The SSP model enables qualitative predictions for conduction $(T(0) \neq 0)$ or insulation $(T(0) = 0)$ at the Fermi level $(E = 0)$. If the molecular graph is a connected–sum Z or edged connected–sum $Z + e$, the multiplicity sequence of the MED, with terminal vertices $\bar{L}$ and $\bar{R}$, which are 0–cfv in the root graphs, can take one of the following sequences:

$$\begin{array}{lllll}
(\eta, & \eta, & \eta, & \eta) & : \text{MED is a conductor or an insulator;} \\
(\eta, & \eta - 1, & \eta - 1, & \eta - 1) & : \text{MED is a conductor;} \\
(\eta, & \eta, & \eta, & \eta + 1) & : \text{MED is a conductor;} \\
 & & & & \\
(\eta, & \eta - 1, & \eta - 1, & \eta) & : \text{MED is a conductor.}
\end{array}$$

If, on the other hand, the terminal vertices in the root graphs are 0–cv, then we can distinguish between connected sum Z and edged-connected sum $Z + e$. The multiplicity sequence can take one value for the connected sum Z and a different value for the edged-connected sum $Z + e$, as follows:

$$\begin{array}{llllll}
\text{Connected Sum } Z: & (\eta, & \eta - 1, & \eta - 1, & \eta - 2) & : \text{MED is an insulator;} \\
 & & & & & \\
\text{Edged-C-Sum} Z + e: & (\eta, & \eta + 1, & \eta + 1, & \eta) & : \text{MED is a conductor.}
\end{array}$$

We end with the result discussed above.

Theorem 6.1. *If the terminals of a MED which is a connected–sum Z or an edged connected–sum $Z + e$ are cv in the root graphs, then the electrical behaviour can distinguish between the two. If the MED is an insulator, then it is a connected–sum Z. If it is a conductor, then it is a an edged–connected–sum $Z + e$.*

It is interesting to note that if a connected–sum Z or an edged connected–sum $Z + e$ happens to have more than one pair of terminal cv vertices that satisfy the definition of its construction from root graphs, and both conduction and insulation occur as the terminals are changed, then the same molecule can act as a switch. The molecule is Z for insulation and $Z + e$ for conduction.

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