

# Eigen-Persistence in Graphs

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## Abstract

The idea of eigen-solution "persistence" from a suitable subgraph into a parent (molecular) graph  $G$  are formalized, in different ways for different cases. Most of it is based on the identification of suitably separated subgraphs sharing common eigenvalues, such that the subgraphs are all isomorphic. We recall Hall's embedding method to identify adjacency-matrix eigen-solutions of a graph  $G$  as persistent from suitable disjoint subgraphs. General rigorous results are obtained for special embeddings, including cases where the subgraphs need not be isomorphic, but rather only share common eigenvalues. The question of accidental degeneracies is addressed, as well as the role of some sort of "local symmetries". Especially the mode of interconnection amongst a suitable family of subgraphs is addressed.

## 1 Preview & framework

Graph eigen-solutions have been a long-considered topic [1–3]– with some early attention to isospectral pairs of graphs. Indeed there has been much study of isospectrality (e.g. [4–16] and many more), though there are several other interesting regularities. Some attention has been directed to the occurrence of excessive (eigenvalue) degeneracies [17–23], sometimes

viewed as manifestations of "local" structures [24–32]. Since degeneracies arose early on in the context of symmetry (and group theory), there has been a natural effort [33–39] to investigate excessive degeneracies in terms of symmetries, most simply in terms of a graph's automorphism group, which generally goes beyond standard point-group symmetries. The much studied [40–45] eigen-solution to the "Bethe tree" manifests high degeneracies. The more general related class of dendrimers also has been much studied, both experimentally [46–51] & theoretically [52–57] - with the theory revealing high degeneracies for the associated adjacency matrices, though often the associated high degeneracies are not noted. Another special topic concerns eigen-features of a subgraph "persisting" up to the parent graph (containing the subgraph), such work appearing (seemingly first) with George Hall [58–60] (and others [61–63]), framing his ideas in terms of "local" reflection symmetries. Many of these special topics relate back further to an earlier topic of null-eigenvalue eigenstates of a graph, as addressed with C. H. Longuet-Higgins (simple) [65] "0 sum rule". This & a host of other early works are discussed in [1–3].

The ideas of degeneracy & symmetry are in fact very fundamental to quantum theory in general. From the very first, degeneracy was noted for the H atom, manifesting an  $SO(4)$  accidental symmetry [65] (beyond  $O(3)$ ) and accounting for the degeneracy of the different angular momenta  $l = 0 \rightarrow n$  found in the quantum solutions [66,67] similar ideas apply [68] for the harmonic oscillator. And there is the von Neumann-Wigner non-crossing rule [69,70], somewhat generally forbidding accidental degeneracies - and being useful far beyond the original case of diatomic potential-energy curves, say to the Woodward-Hoffmann [71] orbital-symmetry conservation rules. Overall such ideas are relevant to correlation diagrams, indicating symmetry relations - see, e.g., [72,73]. Here we address questions of degeneracy & symmetry in the special context of simple graphs.

Inter-relations amongst different eigen-persistences are addressed here, most all concerning special (finitistic) modes of interconnection amongst subgraphs in a parent graph. Attention is directed to eigen-features of subgraphs persisting to the parent graph. The present results seek to unify disparate earlier results, especially on persistence & excessive degeneracy.

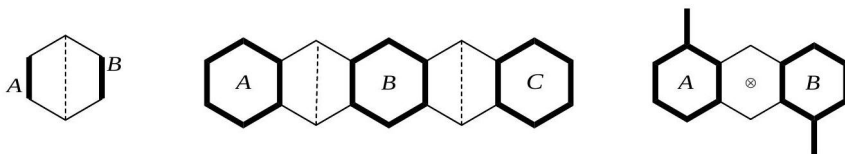
We use graph-theoretic notation, with a graph  $G$  specified by its set  $V(G)$  of vertices and a set  $E(G)$  of edges connecting pairs of vertices. Then  $G$  is labelled by the members of  $V(H)$ , and each edge is labelled by an unordered pair of distinct vertices. A graph  $H$  is a subgraph of  $G$  if  $V(H) \subseteq V(G)$  and  $E(H) \subseteq E(G)$ . Such a subgraph is induced if every edge of  $G$  between two vertices of  $H$  is also an edge in  $H$ . Two graphs  $H$  &  $K$  are isomorphic if there is a one-to-one (bijective) correspondence  $\phi : V(H) \leftrightarrow V(K)$  which also gives a bijection between  $E(H)$  &  $E(K)$ . There is a space spanned by a basis of (orthonormal) vectors, each identified to a vertex  $x \in V(G)$ , and denoted  $|x\rangle$ . A graph  $G$  then has an adjacency operator  $\mathbf{A}_G$  which acts on each  $|x\rangle$  to give a simple sum over  $|y\rangle$  for  $y$  adjacent to  $x$  (that is, for  $y$  with  $\{x, y\} \in E(G)$ ). The operator  $\mathbf{A}_G$  (or associated matrix) has eigen-solutions

$$\mathbf{A}_G |\lambda, Gi\rangle = \lambda |\lambda, Gi\rangle \quad (1)$$

With eigenvalues  $\lambda$ , for which there is a positive integer number  $g(\lambda, G)$  of independent eigenvectors  $|\lambda, Gi\rangle$ , with  $i$  distinguishing any independent (& orthonormal) solutions. The multi-set of eigenvalues (for independent eigenvectors) is called the eigen-spectrum to  $G$ .

A recollection of Hall's work is nice preparation. His fragmentive approach (to eigen-persistence) uses "reflective" embeddings within the parent graph. For instance, for the benzene 6-cycle  $G = C_6$  there is a vertical reflection along the central dashed line as in figure 1. This inter-changes 2-vertex ethylene units  $A$  &  $B$ , for each of which there are two eigen-states  $|\pm, A\rangle$  &  $|\pm, B\rangle$  with eigenvalues  $\pm 1$ . Choosing the upper vertex of each ethylene to have a + amplitude in each of these eigenfunctions, one may verify that  $|+, A\rangle - |+, B\rangle \equiv |+, AB\rangle$  has an amplitude = 0 at the bridge sites between the ethylene subunits, so that there results a benzene eigenstate with eigen-value +1 and  $|-, A\rangle - |-, B\rangle \equiv |-, AB\rangle$  is an eigenstate of benzene with eigen-value -1. Thus the ethylene eigenspectrum is embedded in the benzene eigen-spectrum. Such is usually viewed as a consequence of  $G = C_6$  symmetry diagonalization for a  $\mathcal{D}_6$  group symmetry. Hall's argument extends to pentacene as in the second part of figure

1, where the "local" reflections certainly do not represent (global) automorphisms. Here if  $|\lambda, A\rangle, |\lambda, B\rangle, |\lambda, C\rangle$  eigenvectors (of eigenvalue  $\lambda$ ) are reflected into one another by the local reflections, then the combinations  $|\lambda, A\rangle - |\lambda, B\rangle + |\lambda, C\rangle$  survive as eigenfunctions of pentacene. Notably the local symmetry operations should not be local inversions, as in the third case in figure 1. (There the sites of A & B neighboring a site in the center ring are not symmetry equivalent, and so should not have correspondent amplitudes.)



**Figure 1.** First a  $C_6$  benzene graph, with a vertical dashed line indicating the location of a reflection interchanging the two bold-face "ethylene" subgraphs. Second a pentacene graph with three bold-face benzenes, with dashed lines locating "local" reflections, of just the two near bold-face benzenes. Third, a graph with a center of inversion between two benzyl-radical fragments (but without eigen-persistence).

## 2 Subgraphs & connectors

Focus is on divisions of a parent graph into suitable disjoint fragment subgraphs, with some additional sites inter-connecting between fragments.

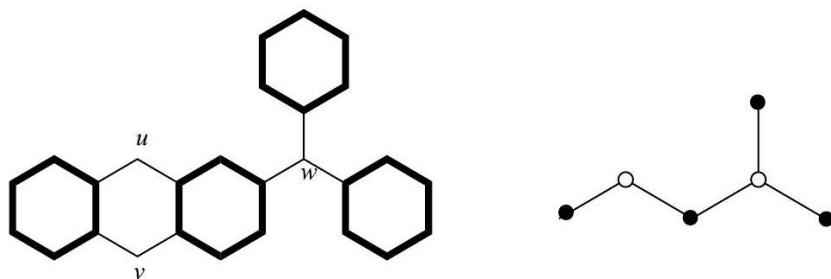
Our eigen-persistence results involve some further ideas. A graph  $G$  is bipartite (or alternant) iff its vertices can be partitioned into two sets  $V_*(G) \& V_o(G)$  such that every edge of  $G$  has one vertex in  $V_*(G)$  & the other in  $V_o(G)$ . Also a subset  $W \subseteq V(G)$  has an (open) neighborhood  $n(W) \equiv \{v \in V(G) : v \notin W, w \in W, \& \{v, w\} \in E(G)\}$ . A subgraph  $H$  is induced iff every pair of vertices in  $V(H)$  which form an edge  $G$  also form an edge in  $H$ .

Now a set  $\mathcal{F}$  of subgraphs is said to be well-separated iff:

- (1) Every  $F \in \mathcal{F}$  is induced and has no intersection with any other  $F' \in \mathcal{F}$ ;

- (2) Every site of  $F \in \mathcal{F}$  occurs in  $n(F')$  for some  $F' \in \mathcal{F}$ ;
- (3) For every pair  $\{F, F'\} \subseteq \mathcal{F}$ , either  $n(F) = n(F')$  or  $n(F) \cap n(F') = \emptyset$ .

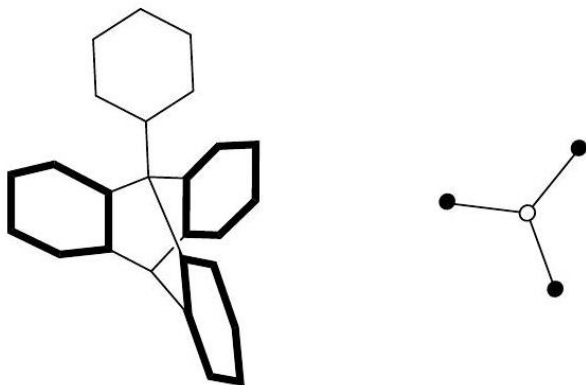
Moreover, given such a well-separated  $\mathcal{F}$  for a graph  $G$ , we say  $n(F)$  an  $m$ -site  $q$ -connector iff first  $m = n(F)$  and second  $q$  is the number of distinct  $F' \in \mathcal{F}$  for which  $n(F') = m$ . An example graph  $G$  is given in figure 2, where the four bold-face benzenes (or hexagons) make-up  $\mathcal{F} = \{F_1, F_2, F_3, F_4\}$ , numbered from left to right, and the set  $\{u, v\} \equiv C_{12}$  is a 2-site 2-connector, while  $\{w\} \equiv C_{234}$  is a 1-site 3-connector. For this example, the eigen-spectrum  $(-2, -1, -1, +1, +1, +2)$  of the bold-face (benzene) hexagons turns out (via later theorems) to persist in  $G$ . In this graph each of the members of  $\mathcal{F}$  are isomorphic subgraphs, but our definition does not demand this, though some of our theorems do. For such a well-separated  $\mathcal{F}$  of  $G$  there is a set  $\mathcal{C}$  of distinct connectors, and an associated derived graph  $G_{\mathcal{F}\mathcal{C}}$  with vertex set  $V(G_{\mathcal{F}\mathcal{C}}) = \mathcal{F} \cup \mathcal{C}$  and edge set  $E(G_{\mathcal{F}\mathcal{C}}) = \{F, C\} : F \in \mathcal{F}, C \in \mathcal{C}, n(F) = C\}$ . From the  $G$  in the first part of figure 2, one then obtains the derived graph in the second part of figure 2. Another example is given in figure 3 showing a graph  $G$



**Figure 2.** First a graph  $G$  with benzene fragments of  $\mathcal{F}$  in bold-face. Second, the reduced derived graph, with full dots for benzenes & open dots for connectors.

with a fragment set  $\mathcal{F}$  made up of three bold-face benzenes with a 2-site 3-connector. Its derived graph is also shown, but note that the fourth benzene ring at the top of  $G$  is not part of either  $\mathcal{F}$  nor  $\mathcal{C}$ , and does not register in the derived graph. Still our theorems (to come) indicates

that the benzene eigen-spectrum occurs twice, and that with the ethylene eigen-spectrum (twice in each benzene spectrum) manages to occur 5 times in  $G$  – a 5-fold degeneracy.



**Figure 3.** Another graph, with three bold face benzenes giving  $\mathcal{F}$ , and its derived graph.

In general, the members of  $\mathcal{F}$  are the fragment graphs whose eigenstates & eigenvalues are to persist in  $G$ . For eigenvalue persistence we mean that the identical eigenvalues emerge in the larger "parent" graph, while for eigen-vector persistence we mean that parent-graph eigenvectors relate to that of the subgraph in a "simple way", by taking appropriate combinations of different local subgraph eigenvectors. Generally we seek to choose linear combinations of the eigen-vectors for each fragment  $F_a \in \mathcal{F}$  such that the combination turns out to be an eigenvector to  $G$ . The connection conditions are in terms of a precise characterization of the isomorphisms amongst the  $F_a \in \mathcal{F}$  and how their "neighborhoods" intersect.

### 3 The Hall case

Hall's illustrative approach entailed isomorphic fragments, with a special "local" relation amongst them - so let's specialize to  $m$ -site  $q = 2$ -connectors. In dealing with isomorphism we introduce a separate base graph  $F_0$ , with (bijective) isomorphisms  $\phi_a : V(F_0) \rightarrow V(F_a)$  for each  $F_a \in \mathcal{F}$ . We say that  $\mathcal{F}$  is  $\phi_a$ -Hall-2-connected in  $G$  iff:

- first, all connectors  $q = 2$ , so can be viewed as edges between their connected fragments of  $\mathcal{F}$  viewed as the vertex set of a reduced derived graph  $G_{\mathcal{F}\mathcal{C}\downarrow}$  which is connected and bipartite;
- second, for each edge  $\{F_a, F_b\}$  of  $G_{\mathcal{F}\mathcal{C}\downarrow}$  and  $u \in V(F_0)$  the  $G$ -edges from  $w \in n(F_a) \cap n(F_b)$  to  $F_a$  or  $F_b$  satisfy  $\{w, \phi_a(u)\} \in E(G) \Leftrightarrow \{w, \phi_b(u)\} \in E(G)$ .

Then we have:

**Theorem** (Hall Theorem 0). *Let  $\mathcal{F}$  be a  $\phi_a$ -Hall-2-connected in  $G$ , with base subgraph  $F_0$  and isomorphism  $\phi_a : F_0 \rightarrow F_a$ , for each  $F_a \in \mathcal{F}$ . Let  $\lambda$  be an eigenvalue of  $F_0$ , with  $i$  th eigen-vector  $|\lambda i, F_0\rangle \equiv \sum_u^{\epsilon V(F_0)} C_{u,\lambda i} |u\rangle$ , and for  $F_a \in \mathcal{F}$  eigen-states are  $|\lambda i, F_a\rangle \equiv \sum_u^{\epsilon V(F_0)} C_{u,\lambda i} |\phi_a(u)\rangle$  where  $|\phi_a(u)\rangle$  is the unit vector for vertex  $\phi_a(u)$  of  $F_a$ . Then corresponding eigen-solutions to  $G$  persist as*

$$\sum_{F_a}^{\in V_*(G_{\mathcal{F}\mathcal{C}\downarrow})} |\lambda i, F_a\rangle - \sum_{F_b}^{\in V_0(G_{\mathcal{F}\mathcal{C}\downarrow})} |\lambda i, F_b\rangle \equiv |\lambda i \uparrow G\rangle. \quad (2)$$

*Proof.* A linear combination of the eigenvectors for each  $F_a \in \mathcal{F}$  is sought such that cancellation of amplitudes transferred to the bridge sites of  $E(\mathcal{F})$  occurs when the adjacency matrix of  $G$  is applied to the linear combination. To see that this occurs for our prospective eigenvector  $|\lambda i \uparrow G\rangle$ , we resolve the adjacency matrix  $\mathbf{A}$  for  $G$  as

$$\mathbf{A} = \sum_{F_a}^{\in \mathcal{F}} \mathbf{A}_a + \sum_{\{F_a, F_b\}}^{\in E(G_{\mathcal{F}\mathcal{C}\downarrow})} \mathbf{A}_{ab} + \mathbf{A}_\emptyset \quad (3)$$

where  $\mathbf{A}_a$  is the adjacency operator for  $F_a$ ,  $\mathbf{A}_{ab}$  is the part of  $\mathbf{A}$  connecting between  $n(F_a) \cap n(F_b)$  &  $V(F_a) \cup V(F_b)$ , while  $\mathbf{A}_\emptyset$  is any remaining part of the adjacency operator (say connecting between  $n(F_a) \cap n(F_b)$  or any parts of  $G$  other than  $F_a$  &  $F_b$ ). Evidently  $\mathbf{A}_\emptyset |\lambda i \uparrow G\rangle \equiv 0$ , and moreover,

$$\sum_{F_a \in \mathcal{F}} \mathbf{A}_a |\lambda i \uparrow G\rangle = \sum_{F_a \in \mathcal{F}} \pm \mathbf{A}_a |\lambda i, F_a\rangle = \sum_{F_a \in \mathcal{F}} \pm \lambda |\lambda i, F_a\rangle = \lambda |\lambda i \uparrow G\rangle \quad (4)$$

Next we identify the set  $E_{a \rightarrow b}$  of  $G$ -edges between a connector  $C_{ab}$  and  $V(F_a)$ , thusly  $E_{a \rightarrow b} \equiv \{\{\phi_a(u), w\} \in E(G) : w \in n(F_a) \cap n(F_b)\}$ . Then for  $F_a \in V_*(\mathcal{F}_G)$

$$\mathbf{A}_{ab} |\lambda i, F_a\rangle = \sum_u^{\in V(F_a)} C_{u, \lambda i} \mathbf{A}_{ab} |\phi_a(u)\rangle = \sum_u^{\in V(F_a)} \sum_{\{\phi_a(u), w\} \in E_{a \rightarrow b}} C_{u, \lambda i} |w\rangle \quad (5)$$

and a similar result occurs on application of  $\mathbf{A}_{ab}$  to  $|\lambda i, F_b\rangle$

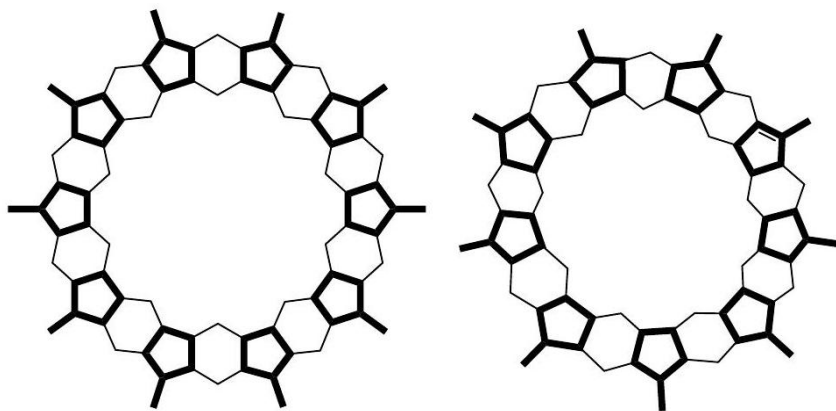
$$\mathbf{A}_{ab} |\lambda i, F_b\rangle = \sum_u^{\in V(F_a)} C_{u, \lambda i} \mathbf{A}_{ab} |\phi_b(u)\rangle = \sum_u^{\in V(F_b)} \sum_{\{\phi_b(u), w\} \in E_{b \rightarrow a}} C_{u, \lambda i} |w\rangle \quad (6)$$

But because of the 3<sup>rd</sup> condition in the definition of Hall-2-connecteness these results for  $\mathbf{A}_{ab} |\lambda i, F_a\rangle$  &  $\mathbf{A}_{ab} |\lambda i, F_b\rangle$  are the same (when  $\{F_a, F_b\} \in E(\mathcal{F}_G)$ ). Thus  $\mathbf{A}_{ab}$  applied to the difference between these two vectors gives 0 (on these  $w \in n(F_a) \cap n(F_b)$ – and overall  $\mathbf{A} |\lambda i \uparrow G\rangle = \lambda |\lambda i \uparrow G\rangle$ . Indeed for different the  $|\lambda i \uparrow G\rangle$  are linearly independent when the  $|\lambda i, F_0\rangle$  are. ■

Note that the definition of Hall-2-connection does not allow the top benzene of figure 3 to be included in  $\mathcal{F}$ . Nor does 3<sup>rd</sup> condition in the definition for Hall-2-connection allow the last graph of figure 1. Most of Hall's examples entailed cases where the derived graphs are trees, whence the bipartiteness is trivial. An example where there are cycles appears in figure 4. The graph on the left has a reduced derived graph  $G_{\mathcal{F} \setminus \mathcal{C} \downarrow}$  which is a 10-cycle  $C_{10}$  while that on the right corresponds to a nonbipartite 9-cycle  $C_9$ . As such the fulvene eigen-spectrum persists for the case on the left, while it does not on the case on right, at least in full completeness. Amusingly the fulvene eigen-solutions for fulvene eigen states which are



odd under the reflection symmetry of a single fulvene fragment survive. The argument uses these 9 odd-symmetry fulvene eigenstates all oriented in the same direction around the 9-cycle, the argument using the simple sum of these 9 odd-symmetry fulvene eigenstates with cancellations occurring in a way like that in the proof above. Thus some further extensions of Hall's ideas are at least partially further extendable.



**Figure 4.** Two cyclic graphs involving pentagon-containing fulvene fragments.

## 4 "Local" symmetries?

Hall's approach surely seems to use a "local" symmetry, and indeed in our associated theorem & proof (and examples) it seems that some sort of symmetries are important. But is this really clear in general? An approach to try to garner understanding in this regard concerns consideration of a reverse problem: given an eigen-state for a parent graph, might there be induced subgraphs from which it could persist?

**Theorem 1.** *Let  $G$  be a connected graph with an eigenvalue  $\lambda$  and eigenvector  $|\lambda, G\rangle$ . Moreover, suppose that the graph left after deletion of all the sites  $x \in V(G)$  where  $|\lambda, G\rangle$  has amplitude = 0 is disconnected. Then the remaining connected subgraphs each have the eigenvalue  $\lambda$ , and eigenvector*

tors which are the projections of  $|\lambda, G\rangle$  onto the sets of sites for each such subgraph.

*Proof.* Let  $A$  be such a connected subgraph, and let  $B$  be the rest of the remaining subgraphic part of  $G$ . Then  $|\lambda, G\rangle$  can be written as a sum of  $|\lambda, A\rangle$  &  $|\lambda, B\rangle$  separately on  $V(A)$  &  $V(B)$ . For projection operators  $O_X \equiv \sum_x^{\epsilon V(X)} |x\rangle\langle x|$ ,  $X \in \{A, B, 0\}$  we have  $|\lambda, A\rangle = O_A|\lambda, G\rangle$ ,  $|\lambda, B\rangle = O_B|\lambda, G\rangle$ , and  $O_0|\lambda, G\rangle = 0$ . Moreover, the adjacency operator may be written as  $\mathbf{A}_G = \mathbf{A}_A + \mathbf{A}_B + \mathbf{A}_0$ , where  $\mathbf{A}_A$  &  $\mathbf{A}_B$  are the adjacency operators for  $A$  &  $B$ , while  $\mathbf{A}_0$  has parts connecting internally within  $V(0) = \{x \in V(G) : \langle x | \lambda, G\rangle = 0\}$  but also parts between  $V(0)$  &  $V(A)$  as well as between  $V(0)$  &  $V(B)$  (but no connections between  $V(A)$  &  $V(B)$ ). Then the eigen-relation for  $|\lambda, G\rangle$  appears as

$$(\mathbf{A}_A + \mathbf{A}_B + \mathbf{A}_0)(|\lambda, A\rangle + |\lambda, B\rangle) = \lambda(|\lambda, A\rangle + |\lambda, B\rangle) \quad (7)$$

or upon projection with  $O_A$  this leads to

$$(O_A\mathbf{A}_A + 0 + O_A\mathbf{A}_0)|\lambda, A\rangle + (O_A\mathbf{A}_A + 0 + O_A\mathbf{A}_0)|\lambda, B\rangle = \lambda|\lambda, B\rangle + 0. \quad (8)$$

But  $O_A\mathbf{A}_0|\lambda, A\rangle = 0$  and  $O_A\mathbf{A}_0|\lambda, B\rangle = 0$ , so that  $O_A\mathbf{A}_A|\lambda, A\rangle = \lambda|\lambda, A\rangle$ . Equivalently  $\mathbf{A}_A|\lambda, A\rangle = \lambda|\lambda, A\rangle$ , so that  $|\lambda, A\rangle$  is an eigenvector (with eigenvalue  $\lambda$ ). If  $B$  is connected the theorem is proved. If  $B$  is disconnected we repeat the argument of the proof till each of the connected pieces of  $B$  into which  $G$  has broken under application of  $\mathbf{A}_G$  are identified to correspond to eigen-solutions. ■

Notably this theorem and its proof implicate fragment eigenstates which persist into the parent graph  $G$ , under a general condition of nodal vertices cutting the parent graph apart. The present point is that there is no hint of a requirement of "local" (or global) symmetry. Thence one further wonders whether local symmetries generally have anything to do with eigen-persistence?

## 5 Simplest connectors: Preparation

To address persistence, one might look at a very simple type of connector, namely a 1-site  $q$  connector. And of these the simplest type might have fragment subgraphs just having a single edge to the connector. Before our main results we first consider a simple sort of graph which could be a fragment connected by a single edge to the rest of the parent graph  $G$ , perhaps thru a connector.

To this end consider a general (parent) connected graph  $H$  which is to be a prospective fragment piece in a larger graph  $G$ . Let have  $H$  a distinguished (root) vertex  $x$ , and an eigenvalue  $\lambda$  with degeneracy  $g(\lambda, H)$  (this being the dimension of the associated eigenspace). Let  $g(\lambda(x)H)$  be the maximum number of linearly independent  $\lambda$ -eigenvectors which have amplitude = 0 at the root site  $x$ . Also let  $g(\lambda x H)$  be the minimum number of linearly independent  $\lambda$ -eigenvectors in an eigenbasis such that they have amplitude  $\neq 0$  at the root site  $x$ . Now  $g(\lambda, H) = g(\lambda x H) + g(\lambda(x)H)$ , but an interesting point is:

**Lemma 2.** *Let  $H$  be a graph with a distinguished (root) vertex  $x$  and an eigenvalue  $\lambda$ . Then  $g(\lambda x H)$  is either = 0 or = 1.*

*Proof.* The result is trivially true if  $g(\lambda, H) = 1$ , so let us proceed to higher values. Consider an orthonormal basis  $\{|\lambda i, H\rangle : i \in \{1, \dots, g(\lambda, H)\}\} \equiv \mathcal{B}_\lambda$  for the  $g(\lambda, H)$ -dimensional eigen-space of  $\lambda$ . If there is no pair with non-zero amplitude at site  $x$ , then our desired result is again trivially true (with  $g(\lambda x H) = 0$ ). So let us imagine that there is a pair of distinct basis vectors  $|\lambda i, H\rangle$  &  $|\lambda j, H\rangle$ , with amplitudes  $\langle x | \lambda i, H\rangle \equiv z_i$  &  $\langle x | \lambda j, H\rangle \equiv z_j$  each of which are  $\neq 0$ , and consider two new eigenvectors

$$|\lambda ij, -\rangle \equiv z_j |\lambda i, H\rangle - z_i |\lambda j, H\rangle \quad \& \quad |\lambda ij, +\rangle \equiv z_i |\lambda i, H\rangle - z_j |\lambda j, H\rangle \quad (9)$$

Clearly these two new eigenvectors are non-zero but have an inner product

$$\langle \lambda ij, - \mid \lambda ij, + \rangle \equiv z_j \langle x \mid \lambda i, H \rangle - z_i \langle x \mid \lambda j, H \rangle = 0 \quad (10)$$

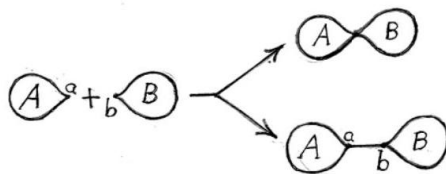
so that they are orthogonal. Upon normalization of each new eigenvector we now have a new orthonormal basis  $\mathcal{B}'_\lambda$  where  $|\lambda i, H\rangle$  has been replaced by (a normalized)  $|\lambda ij, -\rangle$ , while  $|\lambda j, H\rangle$  has been replaced by (a normalized)  $|\lambda ij, +\rangle$ . But this new basis  $\mathcal{B}'_\lambda$  has 1 more basis vector with amplitude = 0 at  $x$ , and 1 fewer basis vectors with  $\neq 0$  amplitude at  $x$ . If  $\mathcal{B}'_\lambda$  has another pair of basis vectors with amplitude  $\neq 0$ , repeat the procedure till finally after a suitable number of repetitions we are left with a basis with but a single eigenvector with non-zero amplitude at  $x$ , whence  $g(\lambda x H) = 1$ . ■

The graph of our lemma might be denoted as one of two initial graphs ( $A\&B$ ) as in figure 5 below, which also shows two different ways to combine these two graphs. The degeneracy notations for its two rooted subgraphs  $A\&B$  parallel that used for the first case of our preceding lemma. That is, when  $A$  has a root  $a$  and an eigenvalue  $\alpha$ , we have degeneracy notations  $g(\alpha, A), g(\alpha(a)A), g(\alpha a A)$ . Similarly for  $B$ , we would have  $g(\beta, B), g(\beta(b)B), g(\beta b B)$ .

Our overall approach seeks to deduce degeneracies in various combined graphs (as in figure 5, but also in other ways, via a 1-site connector, as in the following section). The resultant degeneracies of the combined graphs are implied by theorems, and others not so dictated are here termed accidental. Some of the equalities here will depend on such accidental degeneracies not occurring and will be identified with a funny equal sign  $\approx$ . That is, when this sign  $\approx$  appears, it means that there is equality under the assumption of no such accidental degeneracies for the combination graph.

**Corollary 3.** *Let  $G$  be a graph as one of the two final composite ones in figure 5, where subgraphs  $A\&B$  share an eigenvalue  $\lambda$ . Then  $G$ , also has an eigenvalue  $\lambda$  with degeneracy  $g(\lambda, G) \approx g(\lambda(a)A) + g(\lambda(b)B)$ .*

*Proof.* This is fairly straight-forward, since the eigenvectors of  $A\&B$  with 0 - amplitude at  $a\&b$  are themselves also eigenvectors of  $G$ . ■



**Figure 5.** Two ways of combining two graphs  $A$  with (root site)  $a \in V(A)$  and  $B$  with (root-site)  $b \in V(B)$ .

## 6 1-site 2-connectors

We continue with the consideration of eigen-persistence, as arise from simple 1-site 2-connectors, each fragment subgraph connected by but a single edge to the rest of the parent graph. Another 1-site connector to 3 graphs is indicated in the second part of figure 6, though in this section we only consider the first situation where the fragments are edge connected via a single edge, we return to the 3-connector case in the next section.



**Figure 6.** Patterns to generate from two ( $A \& B$ ) a new graph via one 2-connector, or from three ( $A, B, C$ ) graphs a new graph via a single-site 3-connector.

**Theorem 4.** *Let  $G$  be as in figure 6. where subgraphs  $A \& B$  share an eigenvalue  $\lambda$ . Then  $G$  has an eigenvalue  $\lambda$ , with degeneracy  $g(\lambda, G) \approx g(\lambda(a)A) + g(\lambda(b)B) + g(\lambda a A)g(\lambda b B)$ .*

*Proof.* From the observation that the eigenvectors of  $A \& B$  with 0 amplitude are themselves also eigenvectors of  $G$ , one sees that there is always a  $g(\lambda(a)A) + g(\lambda(b)B)$  contribution. But for the very limited choices for  $g(\lambda a A) \& g(\lambda b B)$ , there but few different cases to consider, as is convenient to do in terms of a tabulation, to identify the different possible total de-

degeneracies  $g(\lambda, G)$ . This tabulation with  $g(\lambda aA)$  &  $g(\lambda aA)$  abbreviated to  $\alpha$  &  $\beta$ , then appears as in table 1. Here beyond the contribution from sub-

$g(\lambda aA)$	$g(\lambda bB)$	$g(\lambda(a)A)$	$g(\lambda(b)B)$	$g(\lambda, G)$
1	1	$\alpha - 1$	$\beta - 1$	$(\alpha - 1) + (\beta - 1) + 1 = \alpha + \beta - 1$
0	1	$\alpha$	$\beta - 1$	$(\alpha - 1) + (\beta) = \alpha + \beta - 1$
1	0	$\alpha - 1$	$\beta$	$(\alpha) + (\beta - 1) = \alpha + \beta - 1$
0	0	$\alpha$	$\beta$	$\alpha + \beta = \alpha + \beta$

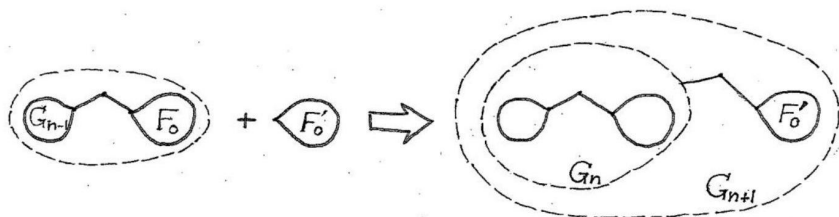
**Table 1.** Degeneracies in proof of theorem 4.

graph eigenstates with 0 amplitude at the root sites  $a$  &  $b$ , one can also obtain a further (single) eigenvector if both  $A$  &  $B$  have an eigenvector counted by  $g(\lambda aA) \cdot g(\lambda bB) = 1 \cdot 1 = 1$ . That is, if  $|\lambda_i, A\rangle$  &  $|\lambda_j, B\rangle$  have non-aero amplitudes  $\langle x | \lambda_i, A \rangle \equiv z_i$  &  $\langle x | \lambda_j, BG \rangle \equiv z_j$ , then we can define  $|\lambda_{ij}G\rangle \equiv z_j|\lambda_i, A\rangle - z_i|\lambda_j, B\rangle$ , which turns out to have 0 amplitude at the central cut-vertex  $x$ . Thus each of the lines of the table are justified, and we obtain the result of the theorem. ■

This result enables a simple consequence for the possibility of high degeneracies. To see this consider a collection  $\mathcal{F}$  of potential subgraphs each sharing a common eigenvalue  $\lambda$ , and introduce the idea of a single site 2-connection between pairs of graphs  $A$  &  $B$  from  $\mathcal{F}$ , to be connected up via the single-site 2-connection of lemma 2. We can further define a sequence  $S(\mathcal{F})$  of graphs  $G_1, G_2, G_3, \dots$  built up from the graphs of  $\mathcal{F}$  step by step: starting with  $G_1$  as copies of two subgraphs from  $\mathcal{F}$  combined in a single-stie 2-connection as indicated in figure 7, then the sequences continues with  $S(\mathcal{F})$  combined with another copy of some graph from  $\mathcal{F}$  to give  $G_{n+1}$

**Proposition 5.** *Given a collection of potential subgraphs  $\mathcal{F}$  each with a degeneracy  $g_0$  for eigenvalue  $\lambda$ , there one can combine them to form a sequence  $S(\mathcal{F})$  of graphs where the degeneracy of the  $n$ th graph  $G_n$  is  $g_n \geq n \cdot (g_0 - 1) + 1$ .*

*Proof.* We use the hypothesis that each copy from  $\mathcal{F}$  has the same degeneracy  $g_0$  (for eigenvalue  $\lambda$ ). From theorem 3, it is seen that  $g_1$  for the first graph  $G_1$  of the sequence  $S(\mathcal{F})$  gives a degeneracy  $g_1 \equiv g(\lambda, G_1) \geq 2g_0 - 1$ .



**Figure 7.** The manner of iteration to build up a sequence  $G_1, G_2, G_3, G_4, \dots$  of polymer graphs of increasing sizes.

Now for the general induction step, we presume that  $g_m \geq m \cdot (g_0 - 1) + 1$  for  $m < n$ , and see what happens for  $m = n$ . At this stage we have  $G_{n-1}$  combining with some  $F \in \mathcal{F}$  via a single-site 2-connection to give  $G_n$  which via theorem 3 has degeneracy

$$\begin{aligned} g_n &\equiv g(\lambda, G_n) \geq g(\lambda, G_{n-1}) + g_0 - 1 \\ &\geq [(n-1)(g_0 - 1) + 1] + g_0 - 1 = n(g_0 - 1) + 1 \end{aligned} \quad (11)$$

and the proof is completed. ■

As a consequence, it is seen that at least 1 eigen-solution persists (even if  $g_0 = 1$ ). But more generally arbitrarily high degeneracies may be built up, if one starts with an eigenvalue which has a degeneracy  $g_0 \geq 2$ . And moreover this can be done with a multiplicity of different sequences  $S(\mathcal{F})$  depending on not only which members of  $\mathcal{F}$  are selected, but also on how the single-site 2-connections are made. If one builds up sequences by introducing sets  $\mathcal{G}_n$  made from the different possible single-site 2 connections of graphs in  $\mathcal{G}_{n-1}$  starting from  $\mathcal{G}_0 \equiv \mathcal{F}$ , then the build up in degeneracy is exponentially fast.

## 7 1-site 3-connectors

Single-site 3-connection indicated in the second part of figure 6, are of interest too. Indeed such connections were early on recognized in "free

radicals", first identified by Gomberg over a century ago, and reviewed in [74], though many more similarly connected radicaloid, or poly-radicaloid, species [49–51, 75–78]. Their potential for high degeneracies has more recently been emphasized [57] (in the context of "local symmetries"). In fact, the simplest so connected case has been much studied in the case of the so-called Bethe tree [43–45, 79], (often dealing with the Ising model or lattice gas model, rather than the Hückel model) and also a more general class of dendrimers [57]. In our next theorem concerning such connectors, it is useful for a given set of numerical parameters  $\{x_1, x_2, \dots, x_n\}$  to introduce a "multi-parameter delta function"  $\delta(x_1, x_2, \dots, x_n) = 1$  if all  $x_i$  are equal and which  $\delta(x_1, x_2, \dots, x_n) = 0$  otherwise.

**Theorem 6.** *Let  $G$  be a graph where as in figure 8. where subgraphs  $A, B, \& C$  each share an eigenvalue  $\lambda$ . Then  $G$ , also has an eigenvalue  $\lambda$  with degeneracy*

$$g(\lambda, G) \approx g(\lambda(a)A) + g(\lambda(b)B) + g(\lambda(c)C) + \delta(g(\lambda aA), g(\lambda bB), g(\lambda cC), 0). \quad (12)$$

*Proof.* The proof somewhat parallels that of theorem 4, using table 2 now respectively abbreviating  $g(\lambda aA), g(\lambda bB), \& g(\lambda cC)$  to  $\alpha, \beta, \& \gamma$ . Note that there is nothing in these various theorems about isomorphisms between different subgraphs. Here there is a contraction of our previous graphic

$g(\lambda aA)$	$g(\lambda bB)$	$g(\lambda cC)$	$g(\lambda(a)A)$	$g(\lambda(b)B)$	$g(\lambda(c)C)$
1	1	1	$\alpha - 1$	$\beta - 1$	$\gamma - 1$
0	1	1	$\alpha$	$\beta - 1$	$\gamma - 1$
0	0	1	$\alpha$	$\beta$	$\gamma - 1$
0	0	0	$\alpha$	$\beta$	$\gamma$

$g(\lambda, G)$
$(\alpha - 1) + (\beta - 1) + (\gamma - 1) + 2$
$(\alpha) + (\beta - 1) + (\gamma - 1) + 1$
$(\alpha) + (\beta) + (\gamma - 1)$
$(\alpha) + (\beta) + (\gamma)$

**Table 2.** Degeneracies in proof of theorem 6.

consideration, with the understanding that the net result (in the last column) must be of the same form regardless of which members of the sets



of  $g(\lambda aA), g(\lambda aA), g(\lambda cC)$  have the value 0 is independent so long as the number of members = 0 is the same. For the results in the last column, the parenthesied results are for those  $\lambda$ -eigen-solutions comprised from component eigen-vectors with 0 - amplitude on the root sites. As such these last column results are clear for the last two rows. For the next column up, there are just 2 component eigensolutions with 0-amplitude on the root sites, so that what happens is very similar to the 2-component situation in lemma 2 - that is, that there is just a single system  $\lambda$ -eigen-solution involving non-zero amplitudes on the root sites of the so noted 2 components. The case that deserves a little attention is that where there are 3 component-eigen-solutions with a non-zero amplitude on component root sites. Suppose these amplitudes are  $C_a, C_b, C_c$ , so that with the aim to obtain 0 at the central 3-way connection site we need we need the component eigen-states combined with 3 values  $Z_a, Z_b, Z_c$  so that  $z_a C_a + z_b C_b + z_c C_c = 0$ . That is, the two 3-vectors designated by  $\vec{z} \equiv (z_a, z_b, z_c)$  &  $\vec{C} \equiv (C_a, C_b, C_c)$  are orthogonal so that acceptable (linearly independent)  $\vec{Z}$  span only a 2-dimensional space, and a nonparenthesized value of +2 occurs for the case with all the (with and since the re to be orthogonal, there are just 2 independent ones. ■

Now from this theorem we can consider again a sequence  $S(\mathcal{F})$  of polymeric graphs built up via 1-site 2-connectors.

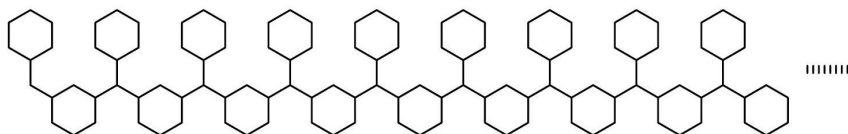
**Proposition 7.** *Given a collection of potential subgraphs  $\mathcal{F}$  each with a degeneracy  $g_0$  for eigenvalue  $\lambda$ , one can combine them via a 1-site 3-copnconnector to form a sequence  $S(\mathcal{F})$  of graphs where the degeneracy of the  $n^{\text{th}}$  graph  $G_n$  is  $g_n \geq 3n \cdot (g_0 - 1/2) + 1/2$ .*

*Proof.* We use the hypothesis that each copy from  $\mathcal{F}$  has the same degeneracy  $g_0$  (for eigenvalue  $\lambda$ ). From theorem 5, it is seen that the first graph  $G_1$  of the sequence  $S(\mathcal{F})$  gives a degeneracy  $g_1 \equiv g(\lambda, G_1) \geq 3g_0 - 1$ . Now for the general induction step, we presume that  $g_m \geq 3m \cdot (g_0 - 1/2) + 1/2$  for  $m < n$ , and see what happens at  $m = n$ . At this stage we have  $G_{n-1}$  combining with some  $F \in \mathcal{F}$  via a single-site 2 -connection to give  $G_n$  which via lemma 2 has degeneracy

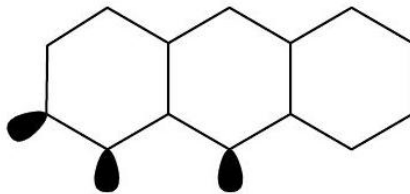
$$\begin{aligned}
 g_n &\equiv g(\lambda, G_n) \geq g(\lambda, G_{n-1}) + 3g_0 - 1 \\
 &\geq [3(n-1)(g_0 - 1/2)] + 3g_0 - 1 = 3(n+1)(g_0 - 1/2) + 1/2
 \end{aligned}
 \tag{13}$$

and the proof is completed. ■

This result means that even starting with graphs with no degeneracy ( $g_0 = 1$ ) such a polymer ends up with a macro-degeneracy (scaling with the number of connector nodes, and polymer length. For instance, the polymer in figure 8 below should have degeneracies associated with the persisting eigenvalues of benzene: of size  $g_n \sim \frac{3}{2}n$  for the (initially nondegenerate)  $\pm 2$  eigenvalues of benzene & of size  $g_n \sim 3n$  for the (initially doubly degenerate)  $\pm 1$  eigenvalues). Moreover, the benzenes with two external connections could have their bonds disposed of in different ways around these benzenes to yield a huge multiplicity of non-regular polymers (with sequences showing identical chemical compositions, but different isomers thereof).



**Figure 8.** Example a (regular) polymer with macro-degeneracies. And as it turns out there are many graphs with eigenvalues of  $\lambda = \pm 2$  or  $\lambda = \pm 1$  so that there is an immense host of possibilities for such sequences  $S(\mathcal{F})$  involving different graphs from  $\mathcal{F}$ . For instance, anthracene (of figure 9) has the benzene eigenvalues (with the same degeneracies (via the Hall theorem) so that inclusion of anthracene in  $\mathcal{F}$  yields many possibilities, with 3 different symmetry inequivalent (chemically plausible) choices of connection-sites on anthracene available (as indicated by little arrows in figure 9).



**Figure 9.** Anthracene with 3 marked vertices.

## 8 Further extensions

The techniques used for proposition 7 fairly readily carry over to a general 1-site  $q$  connector:

**Theorem 8.** *Let  $G$  be a graph  $q$ -connected via a single edge to a root site  $a_i$  of subgraph  $A_i$ ,  $i \in \{1, \dots, q\}$ , each subgraph sharing an eigenvalue  $\lambda$ . Then  $G$ , also has an eigenvalue  $\lambda$  with degeneracy*

$$g(\lambda, G) \approx \sum_{i \in \{1, \dots, q\}} g(\lambda(a_i) A_i) + \delta(g(\lambda a_1 A_1), \dots, g(\lambda a_q A_q), 0). \quad (14)$$

We say that 2 sites  $a$  &  $b$  of a graph  $A$  are automorphically equivalent if there is an automorphism of  $A$  which carries  $a$  to  $b$ . In other nomenclature  $a$  &  $b$  are in the same orbit of  $A$  (under automorphisms of  $A$ ).

**Theorem 9.** *Let  $G$  be a graph  $q$ -connected via  $c_i$  edges to a set of  $c_i$  root sites of subgraphs  $A_i$ ,  $i \in \{1, \dots, q\}$ , such that each root site of  $A_i$  is automorphically equivalent within  $A_i$ . Suppose each subgraph shares an eigenvalue  $\lambda$ , with degeneracy  $g_i$ . Then  $G$ , also has an eigenvalue  $\lambda$  with degeneracy*

$$g(\lambda, G) \geq \sum_{i \in \{1, \dots, q\}} (g_i - c_i + 1) \quad (15)$$

This again is straightforward to prove. But next we look at a few very

special cases.

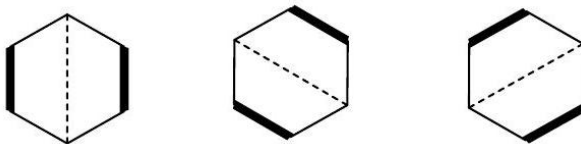
## 9 Miscellaneous commentary

Though we have established more than has previously been set down in a rigorous fashion, there is much which seems not fully developed. The case with many  $q$ -connectors introducing a bipartite derived graph as in our Hall theorem is not fully explored. Also, problems with linear dependences amongst identified degenerate eigenvectors is not yet well illuminated.

### 9.1 Linear dependence problems

The problems with linear independences amongst different associated eigenvectors for different Hall embeddings is conveniently illustrated for benzene. Indeed there are 3 possible reflective cuts for a Hall embedding of ethylenes, as shown in figure 10. Thus there are 3 similar sets of persistent eigenstates - though of the 3 combinations only 2 are linearly independent. (In particular one finds

$|AB, \sigma\rangle + |BC, \sigma\rangle + |CA, \sigma\rangle$  is the 0 -vector, for  $\sigma \in \{+, -\}$ , though also any two of the three like-eigenvalued eigenstates  $|XY, \sigma\rangle$  are independent.) The result is that we expect 2 copies of the ethylene eigenspectrum in benzene. From this it is seen that eigenvalue degeneracies are implicated - and in some cases it might happen that degeneracies beyond that of standard point-group degeneracies (or graph automorphism-group degeneracies) arise - as in the benzenoid of figures 4 & 5.



**Figure 10.** The benzene graph with 3 Hall-embeddings of ethylene.

## 9.2 Cycloacenes illustrate linear dependence problems

There in fact are numerous cases of partial results, for multiple embeddings of the same subgraph. Cyclic poly-acenes turn out to illustrate this in interesting ways - say when there are so many different embeddings that one might wonder just how high degeneracies run. Here "poly-acenes" consist of sequence of hexagons fused together along a "straight" row, with  $N$  hexagons realizing an  $N$ -acene, and if the two ends are fused together in the same fashion one has a cyclo-  $N$ -acene. If  $N = 2M + 2$ , then one may imagine a deletion of the two opposite (outer) sites in two opposite hexagon rings (say rings  $M + 1$  &  $2M + 2$ ), whence there remain two (non-cyclic)  $M$ -acenes. We denote energy-  $\varepsilon$  eigenvectors for these two  $M$ -acenes as  $|1 \rightarrow M, \varepsilon\rangle$  &  $|2M + 1 \rightarrow M + 2, \varepsilon\rangle$  with an orientation such that the ends at the beginnings correspond and the ends at the termini are also correspondent. Then the combination

$$\frac{1}{\sqrt{2}}\{|1 \rightarrow M, \varepsilon\rangle - |2M + 1 \rightarrow M + 2, \varepsilon\rangle\} \equiv |(0, M + 1)\varepsilon\rangle \quad (16)$$

is phase consistent. Since there are  $4M + 2$  sites in an  $M$ -acene, there are  $4M + 2$  choices for the energy  $\varepsilon$  (possibly with an additional degeneracy label). But instead of deleting rings  $2M + 2$  (equivalent to 0) &  $M + 1$ , we could delete rings  $1$  &  $M + 2$ , or  $2$  &  $M + 3$ , or  $\dots$ , or  $M - 1$  &  $2M + 1$  - and each of these would give phase-consistent choices for eigen-vectors for the cyclo- $2M + 2$ -acene. That is we have  $M + 1$  choices for each  $\varepsilon$ , and thus overall we have  $(M + 1)(4M + 2)$  prospective eigen-vectors for the cyclo- $(2M + 2)$ -acene, though in fact there are just  $4(2M + 2)$  linearly independent sets of eigenvectors. Thus there must be a lot of linear dependence amongst these  $(M + 1)(4M + 2)$  phase-consistent eigenstates, at least when  $M$  is large. There might be "accidental degeneracies", and one might even obtain all the eigen-vectors of the cyclo- $(2M + 2)$ -acene. As the  $M$ -acene eigen-solutions are known analytically this can be analytically answered. One could take wave-vector combinations of the different phase-consistent combinations  $\sum_{m=1}^M e^{ikm} |(m, m + M)\varepsilon\rangle$ , and check to see how many non-

zero norms result. Notably no two such non-zero vectors for different wave-vector values  $k$  can be linearly dependent, as they associate to different irreducible representations of the  $(M + 1)$ -fold cyclic group.

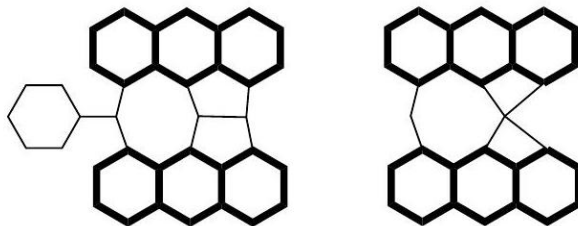
This preceding paragraph applies to cyclo-  $N$ -acenes with  $N$  even. But what about  $N$  odd? For a cyclo-  $N$ -acene (with  $N$  either odd or even), consider deleting the two opposite (outer) sites of one of its rings, say ring  $m$ . Then one is left with a non-cyclic  $(N - 1)$  - acene, with eigen-vectors  $|m, \varepsilon\rangle$ . And of these eigenvectors some number (say  $N_-$ ) of them will be antisymmetric with respect to a reflection interchanging the two ends (at rings  $m - 1$  &  $m + 1$ ). Moreover, each of these is phaseconsistent with itself, so that the eigenvalues associated to such antisymmetric eigen-vectors of  $(N - 1)$  - acenes persist into the cyclo-  $N$ -acene. And as there are  $N$  choices for the ring to be left out, we find  $N$  such persistent eigen-solutions, for each  $\varepsilon$  associated to an antisymmetric  $(N - 1)$  - acene. Clearly (since  $N_-$  scales with  $N$ , and indeed  $N_- \approx 2N$ ) there must generally be a degree of linear dependence which occurs amongst these  $N \cdot N_-$  persistences.

In general one may consider a cyclo-  $L(M + 1)$ -cycloacene and delete  $L$  rings to leave  $L$  noncyclic  $M$ -acenes. If  $L$  is even, then the ideas of the first paragraph in this section are operative, and if  $L$  is odd, then the ideas of the second paragraph here (involving anti-symmetry on the  $M$ -acene fragments) are operative. Overall there seems a degree of degeneracy between cyclo-polyacenes and different sized (quasi-linear) polyacenes. But clearly there are complications with linear dependences.

### 9.3 More examples including beyond 2-connectors

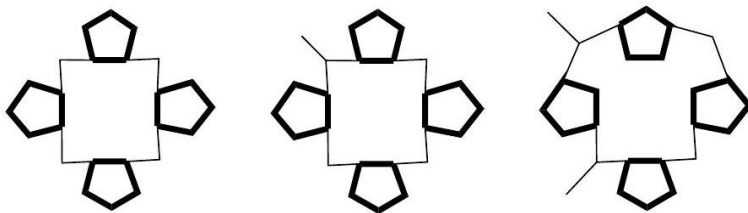
Further examples are given in figure 11, involving Hall-embeddings of anthracene. In the first case, the persistent eigen-solutions identified have a null value on all the sites with no incident bold-face edge. Since anthracene itself Hall-embeds benzene (with manifest double degeneracies for the ethylene eigenvalues), this means that these Hall-embeddings imply that the ethylene eigenvalues occur at least twice in each - in the first diagram the ethylene eigenvalues manifest themselves 3 times due to the extra benzene at the far left, so that triple degeneracies occur.

An example with 4 pentagonal fragment graphs is shown in the first



**Figure 11.** Hall embeddings of the 3-ring anthracene graph.

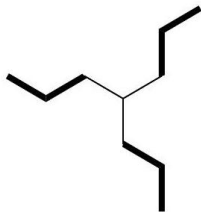
part of figure 12, leading to a pentagon eigen-state & eigen-spectrum being embedded in the is parent graph - with two double degeneracies (inherited from the pentagon. But perhaps double degeneracies do not seem so surprising since the first graph  $G$  has  $C_{4v}$  with 2-dim irreducible representations. However, for the second graph there is just a  $C_\sigma$  reflection symmetry (with this group only having 1-dim irreducible representations) and the last graph has just  $\mathcal{C}_1$ . Still the formal conditions for 2-connected  $\mathcal{F}_G$  still apply, even though in the third case every 2-connection looks different, though the eigen-spectrum (& eigen-solutions) of the pentagon (with 2 double degeneracies) still persist.



**Figure 12.** More 2-connected graphs, still with eigen-persistence, but increasing less symmetry.

Next something covered better in the stuff on 1-site 3-connectors. There are numerous other things which can occur. For instance, an interesting example is found in figure 13. Here one has a 3-fold cyclic symmetry for 3 fragments,  $A, B, C$  and first condition for 2-connectedness of  $\mathcal{F}$  fails. But now one can combine wave-functions of a common eigenvalue ( $\varepsilon$ ) thusly  $|A, \varepsilon\rangle + \eta|B, \varepsilon\rangle + \eta^2|C, \varepsilon\rangle$  with  $\eta \equiv e^{\pm i2\pi/3}$ , to obtain two (degenerate)

wave-functions (one for each choice of  $\eta$ ) for the full graph. This indicates the allyl eigen-spectrum embeds twice into the eigen-spectrum of the overall parent graph - with the result apparently associated to the non-identity irreducible representations of the symmetry with which the parent graph embeds the fragment graphs.



**Figure 13.** A 3-fold symmetric graph.

This 3-fold-symmetric molecule can also be approached using just pairs of allyl subgraphs, whence the 2-connectedness condition for Hall's theorem holds and gives persistences, for 3 different choices of the allyl pairs. The thing which such an approach via Hall's theorem does not reveal is that although the 3 choices lead to 3 choices of persistent eigen-solutions, the triple of eigen-solutions are not independent. The suggested route via a 3-connection seems to lead to linearly independent pairs of persistent eigen-solutions. This triallyl case bears similarity to the biethylene case of benzene as earlier

One might imagine a definition of 3-connectedness somewhat paralleling that of 2-connectedness, still with the connecting intermediate sites adjacent of corresponding sites of the isomorphic (induced) fragment graphs. Indeed, one can imagine even 4-, or general  $m$ -connectedness, whence one gets eigen-spectrum copies corresponding to the non-identity irreducible representations of the symmetric group  $S_m$ . But at the same time the conditions for persistence seem to become more "incomplete" - even though we have strengthened the idea of "accidental eigenvalue-degeneracy" to "eigen-persistence" (including characteristics of associated to both eigenvalues & eigenvectors). Perhaps there is a simpler general formulation?



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## 10 Conclusions

The general notion of eigen-persistence is emphasized, illustrated, and theoretically investigated. A mathematically precise framing of Hall's embedding theorem for the persistence of eigen-spectra of a smaller graph within that of a suitable larger graph is proved. A derived graph plays a crucial role as regards its alternancy. In addition to eigenvalue persistence, we emphasize a type of eigen-vector persistence. But much more has been achieved as regards both persistence and excessive degeneracies. Especially the case of a 1-site  $q$ -connector is dealt with rather generally, where little need of "local" symmetries matters. If there are multiple connectors, there is a derived graph which needs attention. It seems that the weaker the connection between the fully separated fragments, the less the role of local symmetry matters. With more complicated connectors, the more local symmetry helps - at least when supplemented with the presumption of alternancy for the derived graphs. If the members of a family of (eigen-persisting) subgraphs is much relaxed - "restrictive" interconnections seem to contribute to eigen-persistence.

Still many questions remain to do with linear dependences, whence there seem to be multiple (oft linearly dependent) arrangements for subgraphs from which to identify persistences. The general question of eigen-persistence is noticeably strengthened here - but there remains much which is not yet fully clear from a formal general stand-point, as seen in section on "miscellaneous commentary". It seems that with the degree of simplicity in graphs, there arises much "freedom" in the choice of eigenspectra (mediated by the eigen-spaces).

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