Cospectrality-preserving graph modifications and eigenvector properties via walk equivalence of vertices

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Abstract

Originating from spectral graph theory, cospectrality is a powerful generalization of exchange symmetry and can be applied to all real-valued symmetric matrices. Two vertices of an undirected graph with real edge weights are cospectral iff the underlying weighted adjacency matrix $M$ fulfills $[M^k]_{u,u} = [M^k]_{v,v}$ for all non-negative integer $k$, and as a result any eigenvector $\phi$ of $M$ has (or, in the presence of degeneracies, can be chosen to have) definite parity on $u$ and $v$. We here show that the powers of a matrix with cospectral vertices induce further local relations on its eigenvectors, and also can be used to design cospectrality preserving modifications. To this end, we introduce the concept of walk equivalence of cospectral vertices with respect to walk multiplets which are special vertex subsets of a graph. Walk multiplets allow for systematic and flexible modifications of a graph with a given cospectral pair while preserving this cospectrality. The set of modifications includes the addition and removal of both vertices and edges, such that the underlying topology of the graph can be altered. In particular, we prove that any new vertex connected to a walk multiplet by suitable connection weights becomes a so-called unrestricted substitution point (USP), meaning that any arbitrary graph may be connected to it without breaking cospectrality. Also, suitable interconnections between walk multiplets within a graph are shown to preserve the associated cospectrality. Importantly, we demonstrate that the walk equivalence of cospectral vertices $u, v$ imposes a local structure on every eigenvector $\phi$ obeying $\phi_u = \pm \phi_v \neq 0$ (in the case of degeneracies, a specific choice of the eigenvector basis is needed). Our work paves the way for flexibly exploiting hidden structural symmetries in the design of generic complex network-like systems.

Keywords: Cospectrality, symmetric matrices, structure of eigenvectors, matrix powers, walk equivalence

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1. Introduction

Eigenvalue problems of real symmetric matrices are ubiquitous in many fields of science. Special examples are graph theory in mathematics and spectra as well as properties of quantum systems in physics. A first step in dealing with such problems is often based on a symmetry analysis in terms of permutation matrices that commute with the matrix $H$ at hand. Given a set of such permutation matrices, a symmetry-induced block-diagonalization of $H$ is possible and powerful statements about the eigenvectors of $H$ can be made [1, 2]. The permutation symmetries of a matrix can be conveniently visualized in the framework of graphs. A graph representing a matrix $H \in \mathbb{R}^{N \times N}$ is a collection of $N$ vertices connected by edges with weights $H_{i,j}$, like the one shown in Fig. 1. Due to this mapping between a matrix and the graph representing it we denote both the graph and the corresponding matrix with the same symbol $H$. In this graphical picture, the action of a permutation matrix $P$ corresponds to permuting the vertices of the graph, along with the ends of the edges connected to them. $H$ is then transformed to $H' = PHP^{-1}$, and if $P$ and $H$ commute, $PH = HP$, then the graph remains the same after the permutation, i.e. $H' = H$. In particular, if $P$ exchanges two vertices $u$ and $v$, while permuting the remaining vertices arbitrarily, its commutation with $H$
means that the $u$-th and $v$-th row of $H$ coincide, $H_{u,j} = H_{v,j} \forall j \in [1, N] = \{1, 2, \ldots, N\}$ (and the same for the $u$-th and $v$-th column, since $H$ is symmetric). It can then be shown that the $u$-th and $v$-th diagonal elements of any non-negative integer power of $H$ coincide,

$$[H^k]_{u,u} = [H^k]_{v,v} \forall k \in \mathbb{N},$$  

(1)

and that any eigenvector $\phi$ of $H$ has—or, if degenerate to another eigenvector, can be chosen to have—positive or negative parity on $u$ and $v$ [3], that is,

$$\phi_u = \pm \phi_v.$$  

(2)

The eigenvector components on the remaining vertices, which are generally not pairwise exchanged by $P$, may have arbitrary components. Thus Eq. (2) constitutes a local parity of the eigenvectors. This property is intricately related to the interpretation of powers of $H$ in terms of walks [4, 3], which are sequences of vertices connected by edges, on the corresponding graph. For an unweighted graph (having $H_{i,j} \in \{0, 1\}$), the element $[H^k]_{i,j}$ counts all possible walks of length $k$ from vertex $i$ to $j$ on the graph. This is illustrated in Fig. 1 for selected walks of length 1, 2, 3. With this interpretation, Eq. (1)—and thereby also Eq. (2)—hold if the graph has an equal number of “closed” walks starting and ending on $u$ or $v$, for any walk length $k$. This is the case, e.g., for vertices 1 and 2 in the graph of Fig. 1. For weighted graphs (having $H_{i,j} \in \mathbb{R}$), the interpretation of matrix powers in terms of walks is modified by weighing the walks accordingly (see below), with all corresponding results staying valid.

Interestingly, and in many cases counterintuitively, the local parity of eigenvectors of a graph, Eq. (2), can be achieved even if $H$ does not commute with any permutation matrix $P$, as long as Eq. (1) is fulfilled. Given this condition, the eigenvalue spectra of the two submatrices $H \setminus u$ and $H \setminus v$, obtained from $H$ by deleting vertex $u$ or $v$ from the graph, respectively, coincide, and $u$ and $v$ are said to be cospectral [3]. Originating from spectral graph theory [5], the results of the study of cospectral vertices have so far been applied to the field of quantum information and quantum computing, but also—under the term isospectral vertices—to chemical graph theory [6, 7, 8]. In a very recent work [9], cospectral vertices have also been linked to so-called “isospectral reductions”, a concept which allows to transform a given matrix into a smaller version thereof which shares all (or, in special cases, a subset of) the eigenvalues with the original matrix.

Given a graph with cospectral vertices $u$ and $v$, one may ask what kind of changes can be made to it without breaking the cospectrality. One particularly interesting feature that occurs for some graphs is the presence of so-called unrestricted substitution points (USPs), which were introduced in Ref. [8]. Given a graph $H$ with two cospectral vertices $u$ and $v$, a third vertex $c$ is an USP iff one can attach an arbitrary subgraph to $c$ without breaking the cospectrality of $u$ and $v$. While it is a straightforward task to identify all USPs of a given graph, the origin of these special points has been elusive so far.

In this work we shed new light on this phenomenon by introducing the concept of walk equivalence of cospectral vertices $u, v$ with respect to a vertex subset of a graph. In the simplest case of an unweighted graph, two vertices $u$ and $v$ are walk equivalent relative to a vertex subset if the cumulative number of walks from $u$ to this subset equals that from $v$ to this subset, for any walk length. The vertex subset then corresponds to what we call a walk multiplet relative to the pair $u, v$. The smallest walk multiplets, which we call singlets, consist of a single vertex and are identified with the above mentioned USPs, and we here demonstrate how to create such points in a systematic way. Specifically, we show that a graph can be extended via any of its walk multiplets by connecting it to a new vertex while preserving the cospectrality of the associated vertex pair. This procedure can be repeated any number of times with different walk multiplets. All the newly added vertices turn out to be USPs, allowing thus to connect arbitrary new graphs exclusively to them without breaking the cospectrality. Additionally, we show that one can also alter the topology of a graph without extending it by modifying the interconnections between two or more walk multiplets. This provides a systematic way to construct graphs with cospectral vertices but no permutation symmetry, based on breaking existing symmetries by walk multiplet-induced modifications. The concept of walk equivalence of vertices is further generalized to the case where walks to different subsets of a walk multiplet can be equipped with different weight parameters.

Apart from providing means to modify a graph without breaking the cospectrality, we show that walk multiplets can be used to obtain a substantial understanding of the structure of eigenvectors of general real symmetric matrices with cospectral pairs. In particular, for a suitably chosen eigenbasis, walk multiplets induce linear scaling relations between eigenvector components on the multiplet.
vertices, in dependence of the local parity—Eq. (2)—of the eigenvector on the cospectral vertex pair associated with the multiplet. As a special case, the eigenvector components vanish on any walk singlet and, by iteration, on any arbitrary new graph connected exclusively to walk singlets. We believe our work will provide valuable insights into the structure of eigenvectors of generic network-like systems and thereby aid in the design of desired properties.

The paper is structured as follows. In Section 2, we first motivate the concept of walk multiplets as a generalization of USPs, while we define them generally in terms of walks on graphs, and proceed discussing their properties. In Section 3, we show how walk multiplets allow for the modification of graphs without breaking vertex cospectrality. In Section 4, we apply the concept to derive relations between the components of eigenvectors on walk multiplet vertices, with vanishing components on walk singlets as a special case. In Section 5, we use walk multiplets to generate graphs that feature cospectral vertices without having any permutation symmetry. We conclude the work in Section 6. In the Appendix we provide the proofs of all theorems.

2. Walk multiplets

As the name suggests, the concept of “walk multiplets”, to be developed below, is based on walks along the vertices of a graph. In particular, as illustrated in Fig. 1, the entries of powers \( H^k \) can be interpreted in terms of walks [4] on the corresponding graph with \( N \) vertices. Indexing the vertices of the graph by \( v_i \in [1, N] \), a walk of length \( k \) from vertex \( v_i \) to vertex \( v_{k+1} \) is a sequence

\[
\alpha_k(v_i, v_{k+1}) = (v_1, v_2, \ldots, v_k, v_{k+1})
\]

of \( k \) (possibly repeated) edges \( (v_i, v_{i+1}) \) corresponding to nonzero matrix elements \( H_{v_i, v_{i+1}} \). Note that a diagonal element \( H_{v_i, v_i} \) corresponds to a “loop” on vertex \( v_i \), that is, an edge connecting \( v_i \) with itself. If the entries of \( H \) are either 0 or 1, that is, the graph is unweighted, then the element \( [H^k]_{m,n} \) equals the number of walks from \( m \) to \( n \) on the graph. We leave it like this for now, but will consider walks on general weighted graphs further below. Throughout this work \( H = H^\top \in \mathbb{R}^{N \times N} \) will denote a real symmetric matrix but also the corresponding graph itself, since there is a one-to-one mapping between them for our purposes.

2.1. Unrestricted substitution points: the simplest case of walk multiplets

Let us introduce the idea of walk multiplets, starting with some preliminary considerations by inspecting the example graph in Fig. 2 (a), adapted from Ref. [8]. As is common in the field of chemical (or molecular) graph theory, this graph is used as a very simple representation of a molecule with the vertices being atoms of some kind and the edges between them being atom-atom, i.e. molecular, bonds. For simplicity, we consider all bonds to be of the same unit strength, meaning that all edges have the same weight 1, and all atoms to have zero “onsite potential”, so there are no loops on vertices (like the one on vertex 4 in Fig. 1).

While seeming quite common, this graph has some interesting “hidden” properties. First of all, it has cospectral vertices labeled \( u \) and \( v \). This cospectrality does not stem, though, from a corresponding exchange symmetry (permuting vertices \( u \) and \( v \) with each other). Indeed, without being symmetric under exchange, the cospectral vertices fulfill Eq. (1), that is, the number of closed walks from \( u \) back to \( u \) and from \( v \) back to \( v \) is the same, for any walk length \( k \). Notably, cospectral vertices go under the name “isospectral points” in molecular graph theory.

A second interesting property of the graph in Fig. 2 is that it has some special vertices, labeled \( c \) and \( r \), called “unrestricted substitution points” (USPs) [6, 8], which were already mentioned in
Section 1. Those are vertices to which new vertices or subgraphs may be attached, or which may even be removed completely, without breaking the cospectrality of $u$ and $v$. This is done in Fig. 2 (b).

Now, let us approach this in terms of walks, and focus on the vertex $c$ of the example for concreteness. Cospectrality of $u, v$ is preserved when connecting $c$ to the arbitrary new graph $C$, meaning that the number of closed walks from $u$ and $v$ is the same for any walk length also after this modification. 

All additionally created closed walks from $u$ or $v$ which visit the arbitrary subgraph $C$, however, necessarily traverse the USP $c$ on the way. This suggests that the number of walks from $u$ to $c$ is the same as from $v$ to $c$, for any walk length---because the possible walk segments within $C$ are evidently the same for walks from $u$ and from $v$. Indeed, this turns out to be exactly the case: A vertex $c$ of a graph $H$ with cospectral vertices $u, v$ is an USP if and only if it fulfills $[H^1]_{u,c} = [H^1]_{v,c}$ for any non-negative integer $t$.

While already offering a great flexibility, USPs do not necessarily occur in all graphs with cospectral pairs. This leads to the question: Are there other possibilities of graph extensions, involving a set of points instead of just a single point to which one can connect an arbitrary graph? Imagine, for example, a subset $M$ of some graph’s vertex set to which some arbitrary new graph $C'$ can be connected, by connecting an arbitrary single vertex $C'$ of $C'$ to all vertices in $M$, without breaking the cospectrality between two vertices $u, v$ of the original graph. Such a subset $M$, associated in this way with a cospectral vertex pair, corresponds to what we will call a “walk multiplet” relative to $u, v$. An example is illustrated in Fig. 2 (c). The key property, in analogy to USPs, is that the cumulative number of walks from $u$ to all vertices in $M$ is the same as from $v$ to $M$. An USP is then just the simplest case of a walk multiplet consisting of a single vertex, a walk “singlet”.

Below, we will formalize the concept of walk multiplets and describe the various flavors they can assume in general undirected and real-weighted graphs, which correspond to real symmetric matrices. Their value in extending graphs with cospectral vertices will be shown subsequently in Section 3, and their significance for graph eigenvectors will be demonstrated in Section 4. First, we introduce some helpful key notions in the description of walks.

2.2. Weighted walks and walk matrices

Let us first extend the correspondence between walks on a graph, defined in Eq. (3), and powers of its matrix $H$ to a weighted graph, where the entries of $H$ are arbitrary real numbers. Any walk $\alpha_k$ from $v_1$ to $v_{k+1}$ is then given a weight $w(\alpha_k)$ equal to the product of the edge weights $w(v_i, v_{i+1}) = H_{v_i, v_{i+1}}$ of all edges traversed [10], that is,

\[ w(\alpha_k(v_1, v_{k+1})) = w(v_1, v_2)w(v_2, v_3)\cdots w(v_k, v_{k+1}) = \prod_{i=1}^{k}[H]_{v_i, v_{i+1}}. \]  

(4)

The entries $[H^k]_{m,n}$ are then given by the sum over weighted walks as [10]

\[ [H^k]_{m,n} = \sum_{\alpha_k}w(\alpha_k(m,n)) \]  

(5)

where the sum runs over all distinct walks of length $k$ from $m$ to $n$. 

Figure 2: (a) A molecular graph, taken from Ref. [8], which has two cospectral vertices $u, v$ (red) and two “unrestricted substitution points” (USPs) $c, r$. (b) The USPs are vertices which can be connected to any arbitrary graph $C$ (as done with $c$) or also removed from the graph (as done with $r$), without breaking the cospectrality of $u, v$. (c) In the present work we generalize USPs to vertex subsets called “walk multiplets”, an example here being the subset $M = \{m_1, m_2, m_3\}$. We can connect this subset to a new vertex $c'$, which we can in turn connect to an arbitrary graph $C'$, without breaking the cospectrality of $u, v$. The added vertex $c'$ is a walk “singlet”, which is identified as an USP.
Consider, now, a subset \( M \subseteq V \) of the set \( V \) of the vertices of a graph \( H \). The walk matrix of \( H \) relative to \( M \) is the matrix \([e_M, H^2e_M, \ldots, H^{N-1}e_M]\), where \( k \)-th column equals the action of \( H^{k-1} \) on the so called indicator (or characteristic) vector \( e_M \) of \( M \) with \( [e_M]_m = 1 \) for \( m \in M \) and 0 otherwise. Thus, the element
\[
[W_M]_{s,t} = \sum_{m \in M} [H^{t-1}]_{s,m}
\]
equals the sum over weighted walks [in the sense of Eq. (5)] of length \( t - 1 \in [0, N - 1] \) from vertex \( s \) to all vertices of \( M \).

Below we will use this notion of collective walks to vertex subsets to identify structural properties of graphs and their eigenvectors. It will then be convenient, however, to account also for the case where the walks to different vertices \( m \in M \), represented by \([H^{k}]_{s,m}\), are multiplied by some (generally different) factors \( \gamma_m \). Treating \( W_M \) as the Krylov matrix \([12]\) of \( H \) generated by \( e_M \), we thus simply replace this generating vector with a weighted indicator vector \( e_M^\gamma \) having a tuple \( \gamma = (\gamma_m)_{m \in M} \) of general real values \( \gamma_m \) instead of 1’s in its nonzero entries \( m \in M \). This extends the common walk matrix to a corresponding “weighted” version which we denote as \( W_M^\gamma \), that is
\[
W_M^\gamma = [e_M^\gamma, He_M^\gamma, \ldots, H^{N-1}e_M^\gamma], \quad \gamma = (\gamma_m)_{m \in M}, \quad [e_M^\gamma]_m = \begin{cases} \gamma_m, & m \in M; \\ 0, & m \notin M. \end{cases}
\]

For this weighted walk matrix, Eq. (6) is accordingly modified to the more general form
\[
[W_M^\gamma]_{s,t} = \sum_{m \in M} \gamma_m [H^{t-1}]_{s,m}, \quad t \in [1, N],
\]
so that the interpretation of matrix powers in terms of walks is further equipped with weights \( \gamma_m \) for the individual walk destinations \( m \).

### 2.3. Walk equivalence of cospectral vertices

Combining the intuition of equal number of walks to vertex subsets in Section 2.1 with the notion of weighted walk matrices in Section 2.2, it now comes natural to define the general case of a walk multiplet. We will then discuss examples of walk multiplets before analyzing their consequences in the next sections.

**Definition 1 (Walk multiplet).** Let \( H \in \mathbb{R}^{N \times N} \) be a matrix with vertex set \( V \) and walk matrix \( W_M^\gamma \) relative to a subset \( M \subseteq V \) with weighted indicator vector \( e_M^\gamma \) corresponding to the tuple \( \gamma = (\gamma_m)_{m \in M} \). If the \( u \)-th and \( v \)-th rows of \( W_M^\gamma \) fulfill
\[
[W_M^\gamma]_{u,*} = p[W_M^\gamma]_{v,*}
\]
(with * denoting the range \([1, N]\), i.e. all matrix columns), then \( M \) corresponds to an even (odd) walk multiplet with parity \( p = \pm 1 \) relative to the two vertices \( u, v \), denoted as \( M^p_{\gamma;u,v} \) and \( u, v \) are walk equivalent (antiequivalent) with respect to \( M^p_{\gamma;u,v} \).

A walk multiplet \( M^p_{\gamma;u,v} \) is thus not merely a subset \( M \), but this subset equipped with a \([M]\)-tuple of weight parameters \( \gamma \) and a parity \( p \), associated with a given vertex pair \( u, v \). If all weights \( \gamma_m \) are equal, then \( M^p_{\gamma;u,v} \) is a uniform walk multiplet, and we will first discuss such multiplets. In this case the common weight is obviously a global scaling factor in Eq. (9) and can be set to unity without loss of generality, \( \gamma_m = 1 \ \forall \ m \in M \). We will show cases of nonuniform walk multiplets (with unequal \( \gamma_m \) in general) afterwards. Although walk multiplets are generally defined above relative to any pair of vertices \( u, v \), we will concentrate on multiplets relative to cospectral vertices \( u, v \) from now on. Also, for brevity, we will drop the indication of vertices \( u, v \) in the subscript of \( M^p_{\gamma;u,v} \) when they are clear from the context. According to their cardinality (the number \(|M|\) of vertices in \( M \)) we call multiplets “singlets”, “doublets”, etc. Note that the same subset \( M \) can in general correspond simultaneously to different walk multiplets relative to different cospectral vertex pairs or with different tuples \( \gamma \). We should also point out that the notion of “walk equivalence” of two graphs as a whole has been used \([13, 14]\), and stress that we here introduce the notion of walk equivalence of two vertices with respect to a vertex subset.

Before showing examples of walk multiplets, we note that the condition (9) only incorporates walks of length \( k \in [0, N - 1] \) from \( u \) and from \( v \) to \( M \); see Eq. (8). At first sight one might then
preserving the cospectrality of \(\{\gamma\}\) relative to \(\gamma\) values in the tuple partitioned into groups of equal values. We call the vertex subset of a multiplet with such equal weights \(\gamma\) cospectral (among other cospectral pairs) and wonder whether the sum over longer walks \((\gamma = 2)\) walks to different destinations \(m\). Usually, however, those weights \(\gamma\) are not all different from each other, but can be partitioned into groups of equal values. We call the vertex subset of a multiplet with such equal values in the tuple \(\gamma = (\gamma_m)_{m \in M}\) a sublet of the multiplet. In other words, given a nonuniform walk

![Figure 3: (a) A graph with edge weights +1 (solid lines) and −1 (dashed lines) in which the two red vertices \(1\) and \(2\) are cospectral (among other cospectral pairs) and (b) the same graph with edges weighted by 12 real parameters \(w_{u,v}\) as shown, preserving the cospectrality of \(\{1, 2\}\). The tables below list all uniform walk singlets, doublets, and triplets (top to bottom) relative to \(\{1, 2\}\), with superscripts indicating the parity \(p\) of each multiplet; see Example 1.](image)

For an unweighted graph, the notion of walk equivalence of \(u\) and \(v\) with respect to \(M\) then acquires a simple interpretation: An even uniform walk multiplet \((\gamma_m = 1 \forall m \in M)\) corresponds to a vertex subset \(\overline{M}\) such that the number of walks from \(u\) to \(\overline{M}\) equals the number of walks from \(v\) to \(\overline{M}\) (that is, summed over all \(m \in M\)) for any walk length \(k\). Let us now have a look at some uniform walk multiplets in an example graph.

**Example 1.** In the graph depicted in Fig. 3 (a), the two red vertices \(u = 1, v = 2\) are cospectral. All uniform walk singlets, doublets, and triplets of \(H\) with respect to 1, 2 are given in the table below. We put a superscript \(+\) (−) on each individual multiplet subset to indicate its even (odd) parity \(p\). Importantly, the vertex cospectrality and multiplet structure of a graph are in general not strictly bound to a specific set of edge weight values. Indeed, one may generally "parametrize" the edge weights, by setting groups of them to the same but arbitrary real value, and still retain the graph’s vertex cospectrality as well as a subset of its walk multiplets. To demonstrate such a parametrization, in Fig. 3 (b) the graph of Fig. 3 (a) has been weighted by arbitrary real parameters \(w_{u,v}\) \((n = 1, 2, \ldots, 12)\) as shown. The uniform multiplets shown in the table below the graph are present for any choice of the weight parameters \(w_{u,v}\), as does the cospectrality of 1, 2. Note, however, that certain uniform multiplets of the original graph are removed in the parametrized one for arbitrary values \(w_{u,v}\) [that is, if there are no further constraints on these values]; for example, \(\{3, 7\}^+\) and \(\{4, 7\}^+\). Note here that other cospectrality-preserving edge weight parametrizations (not shown) may keep different sets of multiplets intact.

Surely, the graph in Example 1 also features a whole lot of nonuniform multiplets, but we do not show them for simplicity. We have another example dedicated to nonuniform multiplets right below. Apart from that, though, the reader might have noticed that the cospectral pair \(\{1, 2\}\) in Fig. 3 itself is included in the list of uniform walk multiplets. This is not a coincidence for this particular graph.

**Remark 1.** A cospectral vertex pair \(\{u, v\}\) is a uniform even walk doublet relative to itself, since \([H^k]_{u,u} + [H^k]_{u,v} = [H^k]_{v,u} + [H^k]_{v,v}\) with \([H^k]_{u,u} = [H^k]_{v,v}\) by Eq. (1) and \([H^k]_{u,v} = [H^k]_{v,u}\) by the symmetry of \(H = H^\top\). Thus Eq. (10) is fulfilled with \(M = \{u, v\}\) and \(p = +1\).

In the next example, we will illustrate the occurrence of nonuniform walk multiplets, where the walks to different destinations \(m\) in the associated subset \(M\) are generally weighted differently by weights \(\gamma_m\). Usually, however, those weights \(\gamma_m\) are not all different from each other, but can be partitioned into groups of equal values. We call the vertex subset of a multiplet with such equal values in the tuple \(\gamma = (\gamma_m)_{m \in M}\) a sublet of the multiplet. In other words, given a nonuniform walk
The graph in Fig. 4 has two cospectral vertices $a$ and $b$ with corresponding nonzero coefficients $\mu_a = 1$ and $\mu_b = 2$, respectively, where the parameter $a$ can take any nonzero value. Note that the values of sublet coefficients (like $a, b$ in Fig. 4) in different multiplets are unrelated. For instance, $\{4, a, (8)_{-a}\}$ is an even doublet composed of sublets $\{4\}$ and $\{8\}$ with coefficients $a$ and $-a$, independently of the values of $a$ in the other multiplets in Fig. 4. Similarly, $\{(1, a), (3, b), (4)_{a+b}, (5)_{a+b}\}$ is an even quadruplet composed of the four sublets $\{1\}, \{3\}, \{4\}, \{5\}$ with corresponding nonzero coefficients $a, b, 2a + b, a + b$. If, however, any $n > 0$ of these coefficients vanish, then the remaining $4 - n$ sublets with nonzero coefficients constitute a multiplet with $4 - n$ vertices. For example, if $b = -a$, the coefficient of $\{5\}$ vanishes, and the remaining three sublets form the triplet $\{(1, a), (3)_{-a}\}$. Finally, note that any uniform multiplet consists of a single sublet, like, e.g., $\{(1, 4, 7)\}$.
fact, different uniform multiplets may also overlap (that is, have common vertices), and their union is again a multiplet, though a nonuniform one. Take, e.g., the three uniform even multiplets \{(3, 7)a\}⁺, \{(4, 7)a\}⁺, \{(5)a\}⁺, now written with arbitrary uniform weights \(a, b, a′\), respectively. Their union forms the nonuniform even multiplet \{(3)a, (4)b, (5)a, (7)a+b\}⁺ consisting of four sublets with coefficients \(I_{1,2,3,4} = a, b, a′, a + b\). Quite generally, any two walk multiplets of equal parity can be merged into a larger multiplet, as expressed by the following remark.

**Remark 2.** It is clear from Eq. (9) that, if \(A_p^a\) and \(B_p^a\) are two even (odd) walk multiplets with weighted indicator vectors \(e_p^a\) and \(e_p^b\), respectively, then \(C_p^a\) with \(C = A \cup B\) is also an even (odd) multiplet with weighted indicator vector \(e_C^a = e_A^a + e_B^a\).

Note, however, that not all nonuniform multiplets can be decomposed as a union of uniform multiplets. This is easily verified from the table of Fig. 4. For example, the even nonuniform walk quadruplet \((1, 4)_{a'}, (3, 7)b\) is the union of the two even uniform doublets \((2, 6)a\) and \((3, 7)b\), but none of the walk triplets can be decomposed into smaller multiplets (that is, a doublet and a singlet or two overlapping doublets). On the other hand, the nonuniform quadruplet \((1)_{a}, (3)_{−a}, (4)b, (8)_{a−b}\) is composed of the nonuniform triplet \((1, 4)_{a}, (3)_{−a}\) and doublet \((4)_{a'}, (8)_{a−b}\) with \(a′ \equiv b − a\).

### 3. Preserving vertex cospectrality via walk multiplets

Walk multiplets are very valuable for the analysis and understanding of matrices with cospectral vertices \(u\) and \(v\). As we will show, once (one or more of) the walk multiplets of \(H\) relative to \(u\) and \(v\) are known, one can use this knowledge to extend a graph \(H\) by connecting a new vertex (or even arbitrary graphs) to it whilst preserving the cospectrality of \(u\) and \(v\). This naturally generalizes the notion of USPs to subsets of more than one vertex of a graph. We will also show how to interconnect walk multiplets, thereby changing the topology of a given graph, while preserving the associated vertex cospectrality.

In the literature [11], connecting a single vertex to a graph \(H\) via multiple edges of weight 1 results in a graph \(H'\) coined a “cone” of \(H\). To treat general weighted graphs, we will here require cones with weighted edges:

**Definition 2 (Weighted cone).** Let \(H \in \mathbb{R}^{N \times N}\) represent a graph with vertex set \(\mathbb{V} = \{1, 2, \ldots, N\}\). A weighted cone of \(H\) over a subset \(\mathbb{M} \subseteq \mathbb{V}\) with weight tuple \(\gamma = (\gamma_m)_{m \in \mathbb{M}}\) is the graph

\[
H = \left[ \begin{array}{c} \hat{H} \\ e_{\mathbb{M}}^\top \\ e_{\mathbb{M}} \end{array} \right] (13)
\]

constructed by connecting a new vertex \(c = N + 1\) (the tip of the cone) to \(\mathbb{M}\) with edges of weights \(\gamma_m = H_{m,c} = H_{c,m}\) to the corresponding vertices \(m \in \mathbb{M}\), where \(e_{\mathbb{M}}^\top\) is the weighted indicator vector of Eq. (7) with nonzero entries \(\gamma_m\).

For instance, the graph in Fig. 3 (a) is the weighted cone \(H\) over the vertex subset \(\{1, 2\}\) of the graph \(H\ \setminus\ 8\) (\(H\) after removing vertex 8) with weight tuple \(\gamma = (\gamma_1, \gamma_2) = (−1, 1)\). We can now state one of the main results of this work, which will allow for the systematic extension of graphs with cospectral pairs while keeping the cospectrality:

**Theorem 1 (Walk singlet extension).** Let \(H = H^\top \in \mathbb{R}^{N \times N}\) represent an undirected graph with two cospectral vertices \(u, v\), let \(\mathbb{M}^p\) be an even (odd) walk multiplet of \(H\) relative to \(u, v\), and let \(H\) be a weighted cone of \(H\) over the subset \(\mathbb{M}\) with real weight tuple \(\gamma = (\gamma_m)_{m \in \mathbb{M}}\). Then

(i) Vertices \(u, v\) are cospectral in \(H\).

(ii) The tip \(c\) of the cone \(H\) is an even (odd) walk singlet relative to \(u, v\).

(iii) Any even (odd) walk multiplet in \(H\) is an even (odd) walk multiplet in \(H\).

Point (i) of the theorem extends the notion of USPs to vertex subsets for the case of a single new connected vertex \(c\); the vertex \(c\) is now connected to a subset \(\mathbb{M}\) instead of a single USP of a graph without breaking the associated vertex cospectrality. Further, by point (ii) of the theorem, another new vertex \(c'\) can be connected to \(c\) while preserving cospectrality, just as would be the case if \(c\) were a USP. Point (iii) finally allows multiple single new vertices to be connected to different walk multiplets, or to the same walk multiplet. In the case of a USP, however, cospectrality is preserved when connecting a new arbitrary graph to the USP, and not only a single new vertex. This is indeed also the case for a walk singlet.
Corollary 1. Let the vertex $c$ of a graph $H$ be an even (odd) walk singlet relative to a cospectral pair $u, v$ in $H$, and let $C$ be a graph connected exclusively to $c$ via any number of edges with arbitrary weights. Then all vertices of $C$ are even (odd) walk singlets relative to $u, v$.

We thus see that any walk singlet is a USP, and below (Corollary 3) we will also show that the reverse is true. Now, suppose we have connected some walk singlets to corresponding new subgraphs $C, C', \ldots$, which then also consist purely of singlets. Those subgraphs may also be interconnected among each other in an arbitrary manner, by iteratively interconnecting pairs of singlets, leaving the associated cospectrality intact. In fact, vertex interconnections preserving cospectrality can be generalized to the suitable interconnection of arbitrary walk multiplets of equal parity, as ensured by the following theorem.

Theorem 2 (Walk multiplet interconnection). Let $H \in \mathbb{R}^{N \times N}$ be a graph with a cospectral pair $\{u, v\}$ and $X_\gamma, Y_\delta \in \mathbb{R}^\gamma_\delta$ be (in general non-uniform) walk multiplets relative to $\{u, v\}$ having same parity $p$ and weight tuples $\gamma, \delta$, respectively, with possible subset overlap $Z = X \cap Y \neq \emptyset$. Then the cospectrality of $\{u, v\}$ and any walk multiplet relative to $\{u, v\}$ with parity $p$ are preserved in the graph $H \in \mathbb{R}^{N \times N}$ with elements

$$H_{x,y} = H_{y,x} = \begin{cases} \hat{H}_{x,y} + \gamma_x \delta_y & \text{if } x \notin Z \text{ or } y \notin Z \\ \hat{H}_{x,y} + \gamma_x \delta_y + \gamma_y \delta_x & \text{if } x, y \in Z \end{cases} \quad \forall x \in \mathbb{X}, y \in \mathbb{Y}$$

and $H_{i,j} = \hat{H}_{i,j}$, $\forall i, j \notin \mathbb{X} \cup \mathbb{Y}$.

The above theorem, in contrast to the extension of a graph by external vertices in Theorem 1, allows for the internal modification of the graph itself while keeping the cospectrality of a given vertex pair. In particular, the topology of the graph may be changed by adding new edges or deleting existing ones. Before showing examples using Theorems 1 and 2, let us also note the following.

Remark 3. By Theorem 2, one can interconnect a cospectral pair $\{u, v\}$ (which corresponds to a walk doubplet relative to itself) to itself by setting $\mathbb{X} = \mathbb{Y} = \{u, v\}$ and adding an edge between $u, v$ as well as loops on $u, v$, all of equal arbitrary weight (added to possible existing edges), while keeping their cospectrality. Then, by Lemma 3.1 of Ref. [15], those loops can be removed, with $u, v$ still remaining cospectral. In other words, two cospectral vertices $u, v$ of a graph can be interconnected or disconnected without affecting their cospectrality.

To show Theorems 1 and 2 in action, we will now apply them to the example graphs in Fig. 3 (a) and Fig. 4 of the previous section, whose walk multiplet structure has already been analyzed. With the first example, we showcase the cospectrality-preserving extension of a graph: via a uniform walk multiplet, via a combination of overlapping uniform multiplets, and finally by connecting another arbitrary graph to it.

Example 3. In Fig. 5 (a) we have modified the graph of Fig. 3 (a) by connecting a new vertex $c = 9$ to the even uniform walk doubplet $\{3, 7\}^+$ relative to the cospectral pair $\{1, 2\}$ with weight $a$. In the terminology of Theorem 1, this new graph is the cone $H$ of the graph in Fig. 3 (a), $H$ over the subset $\mathbb{M} = \{3, 7\}$ with a weight tuple $\gamma = (\gamma_3, \gamma_7) = (a, a)$. By Theorem 1, vertex $c$ then forms an even singlet and all even multiplets of the graph $H$ in Fig. 3 (a) are still present in the new graph of Fig. 5 (a), as confirmed in the table at the bottom of the figure. Now, in Fig. 5 (b) we further connect $c$ to other vertices in $H$, without breaking the cospectrality of $\{1, 2\}$ or its walk equivalence to any even multiplet. Indeed, by Theorem 2, vertex $c$ can be connected to the even singlet $\{5\}^+$ with some weight $a'$. We can—again by Theorem 2—additionally connect $c$, with weight $b$, to the even uniform doubplet $\{4, 7\}^+$ which overlaps with the already connected one $\{3, 7\}^+$. As a result, the edge $(c, 7)$ now has weight $a + b$. Of course, these successive connections amount to the final graph simply being the weighted cone of the initial one with tip $c$ over $\{3, 4, 5, 7\}$ with weight tuple $\gamma = (\gamma_3, \gamma_4, \gamma_5, \gamma_7) = (a, b, a', a + b)$. Thus, $\{(3)a, (4)b, (5)a', (7)a+b\}^+$ is an even nonuniform walk quadruplet; see Remark 2. In Fig. 5 (c) we make use of Corollary 1 and connect a whole graph $C$, represented by a cloud since it can be just any graph, to the even singlet $c$ via any number of edges with arbitrary weights—again preserving cospectrality and walk equivalence of $\{1, 2\}$. In Fig. 5 (d), we have connected another cloud graph $C'$ to the walk singlet $\{5\}^+$. This latter cloud $C'$ can finally be connected—by Theorem 2—in any arbitrary way to $C$ into a larger cloud graph, since both $\{5\}^+$ and $\{c\}^+$ are even singlets (as are all cloud vertices connected to them). Note that point (iii) of
Figure 5: Extension of a graph via walk multiplets, using Corollary 1 and Theorem 2; see Example 3 for details. The graph of Fig. 3 (a) is successively extended by (a) connecting a new vertex $c = 9$ symmetrically to the even uniform walk doublet $\{3, 7\}^+$ relative to the cospectral pair $\{1, 2\}$ with weight $a$, (b) further connecting $c$ to the even singlet $\{5\}^+$ with weight $a'$ and to the even uniform doublet $\{4, 7\}^+$ with weight $b$, (c) connecting an arbitrary graph $C$ (cloud) to the even walk singlet $c$ via any number of edges with arbitrary weights, and (d) connecting another graph $C'$ to the even walk singlet $\{5\}^+$ and then $C'$ to $C$ in an arbitrary manner, forming a larger arbitrary graph connected to vertices 5 and c. In all steps, the cospectrality of $\{1, 2\}$ as well as the uniform walk multiplets listed in the table below (for up to cardinality 3) are preserved. The graph in (b) is the “weighted cone” of the graph in Fig. 3 (a) over subset $\{3, 4, 5, 7\}$ with weight tuple $\gamma = (\gamma_3, \gamma_4, \gamma_5, \gamma_7) = (a, b, a', a + b)$. Also, $\{(3)_a, (4)_b, (5)_{a'}, (7)_{a+a+b}\}^+$ is an even nonuniform walk quadruplet relative to $\{1, 2\}$ with the same weight tuple $\gamma$.

| $\{5\}^+$, $\{9\}^+$, $\{8\}^{(-)}$ | $\{1, 2\}^+, \{3, 7\}^+, \{4, 7\}^+, \{5, 9\}^+, \{6, 7\}^+$ |
|-----------------------------------|--------------------------------------------------------------------------------------------------|
| $(1, 2)^+, \{3, 5, 7\}^+, \{3, 7, 9\}^+, \{4, 5, 7\}^+, \{4, 7, 9\}^+, \{5, 6, 7\}^+, \{6, 7, 9\}^+$ |                                                                                                                                 |

Theorem 1 means that walk multiplets of the original graph $\hat{H}$ with parity opposite to that of $M^p_\ell$ are not necessarily present in the new graph (cone) $\hat{H}$. Indeed, in the present example with $p = +1$ all but one odd walk multiplet of Fig. 3 (a) (the walk singlet $\{8\}^{(-)}$) disappeared in Fig. 5 (a)–(d).

As we see, using Theorem 1 together with Corollary 1 and Theorem 2, given a graph $H$ with cospectral vertices $u, v$ one can: (1) generate walk singlets by connecting new vertices to existing walk multiplets, (2) connect an arbitrary new subgraph to such a singlet, and subsequently (3) even interconnect such subgraphs. In other words, we now see that, starting from a small graph with cospectral vertices $u$ and $v$, one can construct arbitrarily complex graphs maintaining this cospectrality, using the concept and rules for the introduced walk multiplets.

Let us here also corroborate the necessity of equal parity of two walk multiplets for their combination to be a multiplet (see Remark 2), by a counterexample. In Fig. 5, $\{5\}^+$, $\{8\}^{(-)}$ are walk singlets of opposite parity relative to the cospectral pair $\{1, 2\}$. Assume, now, that these two singlets can be combined into a walk doublet $C^\ell$ relative to $\{1, 2\}$ with subset $C = \{5, 8\}$, weight tuple $c = (a, b)$ and parity $p = \pm 1$. Then, by Theorem 1, connecting a new vertex $c'$ to $C$ via edges with weights $a, b$ would not break the cospectrality. However, this is not the case. Indeed, in the extended graph we would get $[\hat{H}^5]_{1,1} = [\hat{H}^5]_{2,2} - 4ab$, violating Eq. (1) for $k = 5$ if $ab \neq 0$. This means that only one of the vertices $\{5\}^+$ and $\{8\}^{(-)}$ may be connected to $c'$ ($a = 0$ or $b = 0$) to keep $\{1, 2\}$ cospectral. In other words, either even or odd walk multiplets can generally be simultaneously connected to a new vertex while keeping the cospectrality of the associated cospectral pair.

In the following example, we demonstrate how the topology of a graph itself can be modified, i.e. without extending it by new vertices, while preserving a cospectral pair.
Example 4. In Fig. 6, we apply Theorem 2 to the graph of Fig. 4, resulting in graphs with the same vertices as in the original graph but with some of them connected differently. Specifically, in Fig. 6 (a), we interconnect the walk multiplets \((3,7)\) and \((\{1,5\}, \{4,2\})\), with added edge weights as indicated, and in (b) we interconnect walk multiplets \((3,7)\) with \((\{4\}, \{8\})\), starting from the original graph unweighted and setting \(a = 1\).

By Theorem 1, the cospectrality of a vertex pair is preserved in the weighted cone over a walk multiplet of a graph with the same weight tuple \(\gamma\), with the tip of the cone then being a walk singlet.

We now ask for the reverse: When the cospectrality of \(u, v\) is preserved under a single-vertex addition, is that vertex necessarily a walk singlet relative to \(u, v\)? The affirmative answer is given by the following theorem, which also makes a similar statement for the case of single vertex deletions.

**Theorem 3 (Preserved cospectrality under single vertex additions or deletions).** Let \(\hat{H}\) be a graph with vertex set \(\mathcal{V}\) and with two cospectral vertices \(u, v \in \mathcal{V}\). Then

(i) The cospectrality of \(u\) and \(v\) is preserved in the cone \(\hat{H}\) of \(H\) over a subset \(\mathcal{M} \subseteq \mathcal{V}\) with weight tuple \(\gamma = (\gamma_m)_{m \in \mathcal{M}}\) if and only if \(\mathcal{M}_u\) is a walk multiplet relative to \(u, v\).

(ii) The cospectrality of \(u\) and \(v\) is preserved in the graph \(\hat{H} = H \setminus c\) (obtained from \(H\) by removing the vertex \(c \in \mathcal{V}\)) if and only if \(c\) is a walk singlet in \(\hat{H}\) relative to \(u, v\).

Recall that the tip of the cone in part (i) is a walk singlet relative to \(u, v\) (by Theorem 1). In part (ii), a walk singlet is removed, without breaking the cospectrality of \(\{u, v\}\). Thus, the theorem implies that the only way to add a single vertex to a graph, or to remove a single vertex from it, without breaking the cospectrality of two vertices \(u, v\), is if that vertex is a walk singlet relative to \(u, v\). A word of caution, though: Whereas walk singlets can safely be removed from a graph without destroying the associated cospectral pair, the same is not true for larger walk multiplets in general. Combining Theorem 1 with Theorem 3 results in the following conclusion regarding walk singlets.

**Corollary 2.** A vertex \(c\) of a graph is a walk singlet relative to cospectral vertices \(u, v\) if and only if it is exclusively connected via edges with weight tuple \(\gamma = (\gamma_m)_{m \in \mathcal{M}}\) to a walk multiplet \(\mathcal{M}_c\) relative to \(u, v\).
Let us now make the link to where we started (in Section 2.1), with the notion of USPs. Recall that an USP is a single vertex to which an arbitrary new graph can be connected, or which can also be removed, without breaking the cospectrality of a vertex pair. While it is clear from Theorem 1 that any walk singlet is an USP, one might ask if also the reverse is true, that is, whether any USP is a walk singlet. The removal of a walk singlet is covered by Theorem 3 (ii). Regarding the connection of arbitrary graphs, we have the following.

**Corollary 3 (USPs are singlets).** If the cospectrality of a vertex pair \( \{u, v\} \) of a graph \( H \) is preserved when connecting an arbitrary graph \( C \) to a single vertex \( c \) of \( H \), via edges of arbitrary weights, then \( c \) is a walk singlet relative to \( \{u, v\} \).

This statement can be easily understood from the above. Indeed, since \( C \) is an arbitrary graph, we can choose it to be a single vertex \( c' \). If the cospectrality of \( u, v \) is preserved under this addition, then by Theorem 3 (i), \( c' \) must then be a walk singlet. But by Corollary 2, \( c \) must be a walk singlet as well. Thus, we have that every USP is a walk singlet.

Before we proceed, let us review the above, starting with a recapitulation of the concept of cospectral vertices. Known in molecular graph theory as “isospectral points”, this concept can be seen as a generalization of exchange symmetry [6]. Indeed, any two vertices \( u \) and \( v \) that are exchange symmetric are also cospectral, but the reverse is not necessarily the case. Similar to the case of exchange symmetries, one can then draw powerful conclusions from the presence of cospectral vertices. For example, one can use the presence of cospectral vertices to express the characteristic polynomial of the underlying matrix \( H \) in terms of smaller polynomials [16]. In quantum physics it has been shown [3] that cospectrality of \( u \) and \( v \) is a necessary condition for so-called perfect state transfer between these two vertices, which is important in the realization of quantum computers. In general, if two vertices \( u \) and \( v \) are cospectral, then all eigenvectors have (in the case of degeneracies, can be chosen to have) definite parity on these two vertices [15]. The implications of such local parity depend, of course, on what the underlying matrix \( H \) represents, but can be quite impactful. In network theory [9, 17], for example, the local parity of eigenvectors implies that two cospectral vertices have the same “eigenvector centrality”, which is a measure for their importance in the underlying network.

Irrespective of these powerful implications of cospectrality, however, one might object that fulfilling its defining Eq. (1) is rather difficult, especially in larger graphs comprising thousands of vertices. What we have shown above is that fulfilling Eq. (1) is, on the contrary, rather easy: Given a small graph \( G \) with cospectral vertices \( u \) and \( v \), one can easily embed \( G \) into a (much) larger graph \( G' \) by suitably connecting some vertices of \( G' \) to the walk multiplets of \( u \) and \( v \). In other words, we have shown that cospectrality does not necessarily rely on global fine-tuning. This viewpoint-changing finding, however, is just the implication of a much more important insight. Namely, that the matrix powers of \( H \)—which are used to identify walk multiplets—are a source of detailed information about the underlying graph, as we will demonstrate in the following.

4. **Eigenvector components on walk multiplets**

Having seen how multiplets can be used to extend a graph whilst keeping the cospectrality of vertices, we now analyze their relation to the eigenvectors of \( H \). To this end, we first choose the orthonormal eigenvector basis according to the following Lemma.

**Lemma 1 (Lemma 2.5 of [15]).** Let \( H \) be a symmetric matrix, with \( u \) and \( v \) cospectral. Then the eigenvectors \( \{\phi\} \) of \( H \) are (or, in the case of degenerate eigenvalues, can be chosen) as follows. For each eigenvalue \( \lambda \) there is at most one eigenvector \( \phi \) with even local parity on \( u \) and \( v \), i.e., \( \phi_u = \phi_v \neq 0 \), and at most one eigenvector \( \phi \) with odd local parity on \( u \) and \( v \), i.e., \( \phi_u = -\phi_v \neq 0 \). All remaining eigenvectors for \( \lambda \) fulfill \( \phi_u = \phi_v = 0 \). The even (odd) parity eigenvector can be found by projecting the vector \( e_u \pm e_v \) onto the eigenspace associated with \( \lambda \).

**Remark 4.** If the projection of \( e_u \pm e_v \) onto the eigenspace associated with \( \lambda \) yields the zero-vector, then the corresponding even (odd) parity eigenvector does not exist.

With this choice, the components of odd and even parity eigenvectors on a walk multiplet obey the following constraint.

**Theorem 4 (Eigenvector components on walk multiplets).** Let \( H = H^T \in \mathbb{R}^{N \times N} \) represent a graph with a pair of cospectral vertices \( u, v \), and let its eigenvectors be chosen according to
Lemma 1. Then any eigenvector $\phi$ of $H$ with eigenvalue $\lambda$ and nonzero components of odd (even) parity $p$ on $u, v$,

$$\phi_u = p \phi_v \neq 0, \quad p \in \{+1, -1\}, \quad (14)$$

fulfills

$$\sum_{m \in \mathcal{M}} \gamma_m \phi_m = 0 \quad (15)$$

if and only if $M_c^{-p}$ is a walk multiplet relative to $u, v$ with even (odd) parity $-p$ and weight tuple $\gamma = (\gamma_m)_{m \in \mathcal{M}}$.

Remark 5. It is an interesting—and to the best of our present knowledge unanswered—question whether analogous general statements can be made regarding the eigenvector components on walk multiplets relative to a cospectral pair $\{u, v\}$ for eigenvectors with zero components on $u, v$.

Let us take a look at the impact of Theorem 4 in an example. We use a graph we are already familiar with and which has an interesting multiplet structure.

Example 5. The graph of Fig. 4 has three eigenvectors $\phi^\nu$ (labeled by $\nu = 1, 2, 3$) with odd parity on the cospectral pair $\{2, 6\}$; given by the columns

$$
\begin{bmatrix}
-\frac{2}{\sqrt{10}} & \frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\
\frac{1}{\sqrt{10}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
\frac{1}{\sqrt{10}} & \frac{1}{20} \left(5 + \sqrt{5}\right) & \frac{1}{20} \left(5 - \sqrt{5}\right) \\
\frac{1}{\sqrt{10}} & \frac{1}{20} \left(5 - \sqrt{5}\right) & \frac{1}{20} \left(5 + \sqrt{5}\right) \\
0 & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{1}{\sqrt{10}} & \frac{1}{20} \left(-5 - \sqrt{5}\right) & \frac{1}{20} \left(\sqrt{5} - 5\right) \\
\frac{1}{\sqrt{10}} & \frac{1}{20} \left(\sqrt{5} - 5\right) & \frac{1}{20} \left(5 + \sqrt{5}\right)
\end{bmatrix}
$$

As an example, we apply Theorem 4 for the even walk quadruplet $\{(1)_a, (3)_b, (4)_{2a+b}, (5)_{a+b}\}^+$ (shown in the table of Fig. 4) relative to $\{2, 6\}$. By Eq. (15), each of the above eigenvectors fulfills

$$a\phi_1^\nu + b\phi_3^\nu + (2a + b)\phi_4^\nu + (a + b)\phi_5^\nu = 0; \quad \phi_2^\nu = -\phi_6^\nu \neq 0, \quad \nu = 1, 2, 3, \quad (16)$$

for any values of the parameters $a, b$, as the reader may easily verify. Note that the above eigenvectors also have local odd parity on $\{3, 7\}$. This is again a result of Eq. (15), since $\{(3, 7)_a\}^+$ is an even walk doublet relative to the cospectral pair $\{2, 6\}$, so that $\phi_2^\nu + \phi_6^\nu = 0$ for $\nu = 1, 2, 3$.

For uniform walk multiplets, and especially singlets, Theorem 4 simplifies: If an even (odd) walk multiplet $M_c^p$ relative to $u, v$ is uniform ($\gamma_m = \text{const}$), then $\sum_{m \in \mathcal{M}} \phi_m = 0$ for any eigenvector $\phi$ with odd (even) parity on $u, v$; in particular, $\phi$ has zero component on any even (odd) walk singlet. The zero component of an eigenvector $\phi$ on a vertex $c$ can be understood as a cancellation of weighted eigenvector components in the eigenvalue equation $H\phi = \lambda\phi$, written as

$$\sum_{m \neq c} H_{cm}\phi_m = (\lambda - H_{cc})\phi_c.$$ For $\phi_c = 0$, the sum over components $\phi_m$ on vertices $m$ adjacent (i.e., connected by edges) to $c$, weighted by the corresponding edge weights, vanishes, i.e., $\sum_{m \neq c} H_{cm}\phi_m = 0$. This coincides, though, with Eq. (15) of Theorem 4 for $H_{cm} = \gamma_m$. Further, recall that the components of eigenvectors with parity $p$ on cospectral vertices vanish on walk singlets with opposite parity $-p$. In the light of Theorem 1 (ii) and Corollary 1, this suggests that walk multiplets may be used to construct graphs having eigenvectors with multiple vanishing components, namely on graph extensions consisting only of walk singlets. We demonstrate this in the following example.

Example 6. We start with the graph in Fig. 7 (a), which has no walk singlets (or any other walk multiplets up to size 5, for that matter) relative to its cospectral pair $\{1, 8\}$. The cospectrality of $\{1, 8\}$ is independent of the values of the weights $w_1$ and $w_2$ (indicated by solid and dashed lines), as long as they are nonzero. We can now easily create singlets by symmetrically connecting a new graph $C$, depicted by a cloud in Fig. 7 (b), to the two cospectral vertices 1, 8 via a single vertex $c$ of $C$. This is ensured by Corollary 1 and Theorem 2, with the cospectral pair here simultaneously representing a
singlets relative to the only cospectral pair \{1, 8\} which remains cospectral for any nonzero edge weights \(w_1\) (solid lines) and \(w_2\) (dashed lines). The graph has seven eigenvectors with odd local parity (and nonzero components) on \{1, 8\}. (b) When connecting an arbitrary graph \(C\) symmetrically via a single vertex \(c\) to the cospectral pair \{1, 8\}, which is also a uniform even walk doublet \{1, 8\}†, then by Corollary 1 all vertices within \(C\) are walk singlets relative to \{1, 8\}. The original odd party eigenvectors vanish on all vertices of \(C\).

walk doublet (see Remark 1). The original graph in Fig. 7 (a) has seven eigenvectors with odd parity on \{1, 8\} for any choice of the edge weights \(w_1, w_2 \neq 0\). We note that this number can be deduced by applying the methodology of Ref. [18], wherein the so-called “isospectral reduction” is used to split the graph’s characteristic polynomial into smaller pieces, the orders of which are linked to the number of positive and negative parity eigenvectors. Coming back to the example, we note that each of those seven odd parity eigenvectors has vanishing components on all vertices of \(C\) by Corollary 1 and Theorem 4. Of course, depending on the internal structure of the subgraph \(C\), the total graph may now feature further eigenvectors (not those seven from above) which have zero components on different subgraphs (not \(C\)).

When the subgraph \(C\) is much larger than the original graph of Fig. 7 (a), most of the eigenvector components of the seven odd parity eigenvectors vanish. Eigenvectors with such a property are known as “sparse eigenvectors” [19, 20] in engineering or computer science. Such eigenvectors can also be characterized as “compact”, since they have nonzero components only on a strict subset of the vertex set of a graph \(H\). Indeed, if \(H\) represents a Hamiltonian of a physical system composed of discrete sites (like the atoms in molecular model of Fig. 2), then eigenstates of \(H\) which are strictly confined to a subset of sites are often referred to as “compact localized states” [21, 22] or even “dark states” [23, 24] depending on the context. We have here demonstrated how such compact eigenvectors can be generated for a graph featuring cospectral vertices, by extending the graph via walk multiplets. As a perspective for future work, this may be used to design discrete physical setups with compact localized states or, more generally, network systems with some eigenvectors vanishing on desired nodes.

5. Generating cospectral vertices without permutation symmetry from highly symmetric graphs

Until now, the existence of cospectral vertices has been assumed to be given, and we now come to the question of how to generate such graphs. One possible method is to start from two graphs \(G_1, G_2\) with the same characteristic polynomial (such graphs can be constructed by means of the so-called “Godsil-McKay-switching” from Ref. [25]), and then search for a graph \(H\) such that \(H \setminus u = G_1\) and \(H \setminus v = G_2\). The two vertices \(u\) and \(v\) are then guaranteed to be cospectral in \(H\).

The concept of walk multiplets, as introduced in this work, naturally suggests another scheme for generating graphs with cospectral vertices. Starting from a matrix \(H\) which commutes with a permutation matrix \(P\) which exchanges \(u\) and \(v\) (with arbitrary permutations of the remaining vertices, so that other vertices could be symmetry-related as well), one first identifies the walk multiplets of \(H\) relative to \{\(u, v\}\}. In a second step, \(H\) is changed by either (i) connecting one or more new vertices to (some of) the multiplets having common parity, following Theorem 1, or (ii) interconnecting multiplets by adding edge weights between them, following Theorem 2. Vertices \(u\) and \(v\) remain cospectral under these operations, but the resulting matrix \(H'\) may feature less permutation symmetries than \(H\). Interestingly, \(H'\) could feature no permutation symmetry at all, as we demonstrate in the following examples.

**Example 7.** Figure 8 (a) shows a “ladder” graph with two legs and three rungs. As drawn here, it is symmetric both under a reflection about the horizontal and the vertical axis. As a result of the symmetry about the vertical axis, and among other cospectral pairs, the two central vertices \(u, v\)
are cospectral. Moreover, as a result of the combined horizontal and vertical reflection symmetry, the two pairs \{d_1, d_2\} and \{d_1, d_3\} correspond to even uniform walk doublets relative to \{u, v\}. In Fig. 8 (b), a new vertex \(e\) is connected to \{d_1, d_2\} and another new vertex \(e'\) is connected to \{d_1, d_3\}, with some arbitrary but uniform weights \(a\) and \(b\), respectively. The extension by \(e\) and \(e'\) breaks the previous reflection symmetries in the resulting graph, which in fact features no permutation symmetries at all. By Theorem 1, however, the vertices \(u, v\) remain cospectral. An alternative way to generate a graph with cospectral vertices and no permutation symmetries is shown in Fig. 8 (c).

Here the same original graph is modified by applying Theorem 2: Instead of connecting the two walk doublets \{d_1, d_2\} and \{d_1, d_3\} to added vertices, they are now interconnected to each other. Specifically, the weights \(ab\) are added pairwise to the edges between \(d_1, d_2, d_3,\) and a loop of weight \(2ab\) is added to the overlap \(d_1 = \{d_1, d_2\} \cap \{d_1, d_3\}\). Note that, while the vertex set of the graph remains the same, its topology has now changed by the added edges \((d_1, d_3)\) and \((d_2, d_3)\). Again, the pair \(\{u, v\}\) remains cospectral, while the resulting graph has no permutation symmetry.

**Example 8.** Figure 9 (a) shows again a graph which, as visualized, is vertically and horizontally reflection symmetric and has (among others) two cospectral vertices \(u, v\) and two uniform even walk doublets \{d_1, d_2\} and \{d_1, d_3\} relative to \{u, v\}. We now use Theorem 2 to change the topology of the original graph and subsequently Theorem 1 to further extend it by new vertices, with \(u, v\) remaining cospectral in the final graph where all permutation symmetries are broken. Specifically, in Fig. 9 (b) we interconnect the walk doublet \{d_1, d_3\} to the doublet \{u, v\} by uniformly adding edge weights between their vertices (creating new edges if absent) according to Theorem 2. In Fig. 9 (c) we proceed by connecting a new vertex \(c\) to the doublet \{d_1, d_2\} and another new vertex \(c'\) first to \{d_1, d_3\} and then to \{u, v\} (equivalent to connecting \(e'\) directly to the walk quadruplet \{(d_1, d_3), (u, v)\}). Following Theorem 1. We finally also disconnect \(u\) from \(v\), which leaves them cospectral according to Remark 3.

The highly symmetric base graphs in Examples 7 and 8 were chosen unweighted and without loops for simplicity. Notably, they could easily be enriched by adding loops on their vertices and weighting the edges such that the indicated cospectral pairs \{u, v\} are still present (that is, by respecting the reflection symmetries about the vertical and/or horizontal axes). Then, the extensions and interconnections described above could still be performed, creating weighted graphs featuring cospectral pairs without permutation symmetries.

### 6. Conclusions

Cospectral vertices offer the exciting possibility of eigenvectors of a matrix \(H\) having local parity on components corresponding to cospectral vertex pairs, even without the existence of corresponding permutation matrices commuting with \(H\). Here, we introduced the notion of “walk equivalence” of
two cospectral vertices with respect to a vertex subset of a graph represented by a matrix $H$. Such subsets, corresponding to what we call “walk multiplets”, provide a simple and generally applicable method of modifying a given graph with cospectral vertices such that the cospectrality is preserved. The definition of walk multiplets is based on the entries of the powers of $H$ and can be expressed in terms of so-called walk matrices used in graph theory. As we demonstrate here, the concept of walk multiplets generalizes that of “unrestricted substitution points” (USPs), introduced for molecular graphs, to vertex subsets of arbitrary size: Any arbitrary new graph can be connected, via one of its vertices, to all vertices of a walk multiplet relative to a cospectral pair in an existing graph, without breaking the cospectrality. In fact, USPs turn out to coincide with walk “singlets”, that is, multiplets comprised of a single vertex. We further showed how walk multiplets can be used to derive sets of local relations between the components of an eigenvector with certain parity on a given associated cospectral pair. As a special case, the eigenvector components then vanish on any walk singlet as well as on any graph connected exclusively to walk singlets. This relates to the generation of so-called “compact localized states” in artificial physical setups, also known as “sparse eigenvectors” in other areas of science. We also presented a scheme in which we use walk multiplets to construct a class of graphs having cospectral vertices without any permutation symmetries.

It is important to notice that the analysis performed here applies also to more than two cospectral vertices: For any subset $S$ of cospectral vertices, cospectrality is indeed defined pairwise for any two vertices $u, v \in S$, and thus the walk multiplet framework applies to any such pair. Our results may thus offer a valuable resource in understanding and manipulating the structure of eigenvectors in an engineered network system via its walk multiplets—that is, by only utilizing the powers of the underlying matrix. In particular, the local eigenvector component relations derived here may be systematically exploited to deduce parametric forms of eigenvectors for generic graphs with cospectral pairs; an investigation left for future work.

Let us finally also hint at a possible connection to recent studies of local symmetries in discrete quantum models, which provide relations between the components of general states in the form of non-local continuity equations [26, 27] and may offer advantages for state transfer on quantum networks [18]. In this context, it would be intriguing to explore the possible implications of walk multiplets for the dynamical evolution of wave excitations on general network-like systems.

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Appendix A. Proofs of theorems

We here restate Theorems 1 to 4 together with their proofs.

**Theorem 1 (Walk singlet extension).** Let $\tilde{H} = H^\top \in \mathbb{R}^{N \times N}$ represent an undirected graph with two cospectral vertices $u, v$, let $\mathbb{M}_u^\top$ be an even (odd) walk multiplet of $\tilde{H}$ relative to $u, v$, and let $H$ be a weighted cone of $\tilde{H}$ over the subset $\mathbb{M}$ with real weight tuple $\gamma = (\gamma_m)_{m \in \mathbb{M}}$. Then

(i) Vertices $u, v$ are cospectral in $H$. 

Figure 9: The highly symmetric graph in (a) with (among other pairs) the cospectral vertex pair $\{u, v\}$ is modified by (b) interconnecting the walk doublets $\{u, v\}^+$ and $\{d_1, d_3\}^+$ (according to Theorem 2), and then (c) disconnecting the two cospectral vertices $u, v$ from each other (Remark 3), connecting a new vertex $c$ to the walk quadruplet $\{(d_1, d_3), (u, v)\}^+$ (Theorem 1), resulting in a graph with cospectral vertices $u, v$ but no permutation symmetries; see Example 8.
(ii) The tip $c$ of the cone $H$ is an even (odd) walk singlet relative to $u, v$.

(iii) Any even (odd) walk multiplet in $H$ is an even (odd) walk multiplet in $\hat{H}$.

Proof. We partition any walk of length $k$ in $H$ into the walks restricted exclusively to $\hat{H}$ and the additionally generated walks in $\hat{H}$ visiting the new vertex $c$. Then we apply the multiplet condition, Eq. (10), which is valid in the old graph $\hat{H}$. For convenience, we define

$$B^{(k)}_{u,M} \equiv \sum_{m \in M} \gamma_m [H^k]_{u,m}, \quad (A.1)$$

and similarly $\hat{B}^{(k)}_{u,M}$ for $\hat{H}$. Then, since $M_p$ is a walk multiplet relative to $u, v$ in $\hat{H}$, we have from Eq. (10) that

$$B^{(k)}_{u,M} = p \hat{B}^{(k)}_{v,M} \quad \forall k \in \mathbb{N}, \quad p \in \{+1, -1\}, \quad (A.2)$$

To prove (i), we compute, with walk lengths fulfilling $\ell + n + r = k - 2$,

$$[H^k]_{u,u} = [\hat{H}^k]_{u,u} + \sum_{\ell,n,r} \sum_{m,m' \in M} [\hat{H}^\ell]_{u,m} H_{m,c} [H^n]_{c,\ell} H_{\ell,m'} [\hat{H}^r]_{m',u} \quad (A.3)$$

$$= [\hat{H}^k]_{u,u} + \sum_{\ell,n,r} \sum_{m,m' \in M} [\hat{H}^\ell]_{u,m} \gamma_m [H^n]_{c,\ell} H_{\ell,m'} [\hat{H}^r]_{m',u} \quad (A.4)$$

$$= [\hat{H}^k]_{u,u} + \sum_{\ell,n,r} \hat{B}^{(\ell)}_{u,M} [H^n]_{c,\ell} \hat{B}^{(r)}_{u,M} \quad (A.5)$$

$$= [\hat{H}^k]_{u,u} + p^2 \sum_{\ell,n,r} \hat{B}^{(\ell)}_{v,M} [H^n]_{c,\ell} \hat{B}^{(r)}_{v,M} \quad (A.6)$$

where we used $p^2 = 1$, Eq. (A.2), and the cospectrality of $u, v$ in $\hat{H}$. To prove (ii), we compute, now with $\ell + n = k - 1$,

$$[H^k]_{u,c} = \sum_{\ell,n} \sum_{m \in M} [\hat{H}^\ell]_{u,m} H_{m,c} [H^n]_{c,\ell} = \sum_{\ell,n} \sum_{m \in M} \gamma_m [\hat{H}^\ell]_{u,m} [H^n]_{c,\ell} \quad (A.8)$$

$$= \sum_{\ell,n} \hat{B}^{(\ell)}_{u,M} [H^n]_{c,\ell} \quad (A.9)$$

$$= \sum_{\ell,n} p \hat{B}^{(\ell)}_{v,M} [H^n]_{c,\ell} = p [H^k]_{c,c} \quad (A.10)$$

To prove (iii), we compute, again with $\ell + n = k - 1$,

$$[H^k]_{u,m} = [\hat{H}^k]_{u,m} + \sum_{\ell,n} \sum_{m' \in M} [\hat{H}^\ell]_{u,m'} H_{m',c} [H^n]_{c,m} \quad (A.11)$$

$$= [\hat{H}^k]_{u,m} + \sum_{\ell,n} \hat{B}^{(\ell)}_{u,M} [H^n]_{c,m} \quad (A.12)$$

so that, multiplying by $\gamma_m$ and summing over $m \in M$, we have

$$B^{(k)}_{u,M} = \hat{B}^{(k)}_{u,M} + \sum_{m \in M} \gamma_m \sum_{\ell,n} \hat{B}^{(\ell)}_{u,M} [H^n]_{c,m} \quad (A.13)$$

$$= p \hat{B}^{(k)}_{v,M} + \sum_{m \in M} \gamma_m \sum_{\ell,n} p \hat{B}^{(\ell)}_{v,M} [H^n]_{c,m} \quad (A.14)$$

$$= p \sum_{m \in M} \gamma_m ([H^k]_{v,m} + \sum_{\ell,n} \hat{B}^{(\ell)}_{v,M} [H^n]_{c,m}) = p \sum_{m \in M} \gamma_m [H^k]_{v,m} = p B^{(k)}_{v,M} \quad (A.15)$$

Note that, if any arbitrary graph $C$ is connected exclusively to the added vertex $c$, then any vertex $c'$ of $C$ is also a walk singlet relative to $\{u, v\}$. Indeed, simply replacing $[H^n]_{c,c}$ with $[H^n]_{c,c'}$ in Eqs. (A.8) to (A.10) above leads to $[H^k]_{u,c,c'} = p [H^k]_{v,c'}$, which proves Corollary 1.
Theorem 2 (Walk multiplet interconnection). Let $\tilde{H} \in \mathbb{R}^{N \times N}$ be a graph with a cospectral pair \(\{u, v\}\) and \(\mathbb{X}_\alpha, \mathbb{Y}_\beta\) be (in general non-uniform) walk multiplets relative to \(\{u, v\}\) having same parity \(p\) and weight tuples \(\gamma, \delta\), respectively, with possible subset overlap \(Z = X \cap Y \neq \emptyset\). Then the cospectrality of \(\{u, v\}\) and any walk multiplet relative to \(\{u, v\}\) with parity \(p\) are preserved in the graph \(H \in \mathbb{R}^{N \times N}\) with elements

\[
H_{x,y} = H_{y,x} = \begin{cases} 
\tilde{H}_{x,y} + \gamma_x \delta_y & \text{if } x \notin Z \text{ or } y \notin Z \\
\tilde{H}_{x,y} + \gamma_x \delta_y + \gamma_y \delta_x & \text{if } x, y \in Z 
\end{cases} \quad \forall \, x \in X, y \in Y
\]

and \(H_{i,j} = \tilde{H}_{i,j} \forall \, i, j \notin X \cup Y\).

Proof. To prove that the vertices \(u, v\) remain cospectral in the modified graph \(H\) with added edge weights \(\tilde{H}_{x,y} = \tilde{H}_{y,x}\) as described in the theorem, we will partition the walks in the new graph into walk segments such that the multiplet relations, Eq. (9), can be applied for the segments within the old graph \(\tilde{H}\).

We first express the newly generated closed walks from \(u\) using (i) walks segments in the old graph \(\tilde{H}\) to reach a vertex of one of the multiplets \(X\) (or \(Y\)), (ii) the new edge (that is, the weight added if the edge already existed) to cross to the other multiplet \(Y\) (or \(X\)), and (iii) finally coming back to \(u\) using walks in the new graph \(H\).

Defining \(M = \mathbb{X} \setminus Z, \mathbb{W} = \mathbb{Y} \setminus Z\), and with added edge weights \(H_{ij} - \tilde{H}_{ij} = \gamma_i \delta_j \) (resp. \(\gamma_i \delta_j + \gamma_j \delta_i\)) if \(i, j \in \mathbb{X} \cup \mathbb{Y} \land (i \notin Z \lor j \notin Z)\) (resp. \(i, j \in Z\)), we have

\[
[H^k]_{u,u} = [\tilde{H}^k]_{u,u} + \sum_{l+n+1=k} \left\{ \sum_{m \in M, z \in Z} [\tilde{H}^1]_{u,m} \gamma_m \delta_z [H^n]_{w,u} + \sum_{x \in X, w \in W} [\tilde{H}^1]_{u,z} \gamma_x \delta_u [H^n]_{w,u} \right\} \quad (A.16)
\]

\[
= \sum_{l+n+1=k} \left\{ \sum_{m \in M, z \in Z} [\tilde{H}^1]_{u,m} \gamma_m \delta_z [H^n]_{z,u} + \sum_{x \in X, w \in W} [\tilde{H}^1]_{u,z} \gamma_x \delta_u [H^n]_{z,u} \right\} \quad (A.18)
\]

We can now combine sums over subsets as follows: \(\sum_{m \in M} + \sum_{z \in Z} = \sum_{x \in X}\) in (A.16), and the same in (A.18) with the first term \((\gamma_z \delta_z)\) in (A.20). Similarly, \(\sum_{w \in W} + \sum_{z \in Z} = \sum_{y \in Y}\) in (A.17), and the same in (A.19) with the second term \((\gamma_z \delta_z)\) in (A.20). This yields

\[
[H^k]_{u,u} = [\tilde{H}^k]_{u,u} + \sum_{l+n+1=k} \left\{ \sum_{x \in X, w \in W} [\tilde{H}^1]_{u,x} \gamma_x \delta_w [H^n]_{w,u} + \sum_{y \in Y, m \in M} [\tilde{H}^1]_{u,y} \gamma_y \delta_m [H^n]_{m,u} + \sum_{x \in X, z \in Z} [\tilde{H}^1]_{u,x} \gamma_x \delta_z [H^n]_{z,u} + \sum_{y \in Y, z \in Z} [\tilde{H}^1]_{u,y} \gamma_y \delta_z [H^n]_{z,u} \right\} \quad (A.20)
\]

Next, we account for the walk segments from vertex \(i = x, y\) back to \(u\), which have a similar form:

\[
[H^n]_{i,u} = [H^n]_{i,u} + \sum_{r+s+1=n} \left\{ \sum_{x' \in X, y' \in Y} [H^r]_{i,x'} \gamma_{x'} \delta_{y'} [H^s]_{y',u} + \sum_{y' \in Y, x' \in X} [H^r]_{i,y'} \gamma_{y'} \delta_{x'} [H^s]_{x',u} \right\} \quad (A.22)
\]

Plugging this into (A.21), after some sorting and combining of terms we arrive at (with \(x, x' \in X\) ...
and \( y, y' \in \mathcal{V} \)

\[
[H^k]_{u,u} = [\tilde{H}^k]_{u,u} + 2 \sum_{l+n+1=k} \sum_{x,y} [\tilde{H}^l]_{u,x} \gamma_x \delta_y [H^n]_{y,u} + \sum_{l+r+s+2=k} \sum_{x,x',y,y'} \left\{ [\tilde{H}^l]_{u,x} \gamma_x \delta_y [H^r]_{y,y'} \delta_{y'} \gamma_{x'} [\tilde{H}^s]_{x',u} + [\tilde{H}^l]_{u,y} \delta_y \gamma_{x'} [H^r]_{x',x} \gamma_{x'} \delta_{y'} [H^s]_{y,y'} + 2[\tilde{H}^l]_{u,x} \gamma_x \delta_y [H^r]_{y,y} \delta_{y'} \gamma_{x'} [\tilde{H}^s]_{x',u} \right\}
\]  

(A.23)

It is now evident that \([H^k]_{u,u}\) is equal to \([H^k]_{v,v}\) by applying cospectrality of \( u, v \) in \( \tilde{H} \) and multiplet conditions for \( \mathcal{X}_{p, \gamma}^p \).

To prove that any general non-uniform walk multiplet \( \mathbb{Q}^p \) (with weight tuple \( p \) and of the same parity \( p \) as \( \mathcal{X}_{p, \gamma}^p, \mathcal{Y}_{\gamma}^p \)) in \( \tilde{H} \) is preserved in \( H \), we evaluate the following expression by using Eq. (A.22):

\[
\sum_{q \in \mathbb{Q}} \epsilon_q[H^k]_{u,q} = \sum_{q \in \mathbb{Q}} \epsilon_q\left\{ [H^k]_{u,q} + \sum_{r+s+1=n} \sum_{x,y} [H^r]_{u,y} \delta_y \gamma_{x} [H^s]_{x,q} + \sum_{r+s+1=n} \sum_{y \in \mathcal{V}, x \in \mathcal{X}} [H^r]_{u,x} \delta_x \gamma_y [H^s]_{y,q} \right\}
\]  

(A.24)

\[
= p \sum_{q \in \mathbb{Q}} \epsilon_q[H^k]_{v,q},
\]  

(A.25)

where in the last step we applied the multiplet conditions for \( \mathbb{Q}_c^p, \mathcal{X}_c^p, \mathcal{Y}_c^p \).

\[ \square \]

**Theorem 3 (Preserved cospectrality under single vertex additions or deletions).** Let \( \tilde{H} \) be a graph with vertex set \( \mathcal{V} \) and with two cospectral vertices \( u, v \in \mathcal{V} \). Then

(i) The cospectrality of \( u \) and \( v \) is preserved in the cone \( H \) of \( \tilde{H} \) over a subset \( \mathcal{M} \subseteq \mathcal{V} \) with weight tuple \( \gamma = (\gamma_m)_{m \in \mathcal{M}} \) if and only if \( \mathcal{M}^p_{\gamma} \) is a walk multiplet relative to \( u, v \).

(ii) The cospectrality of \( u \) and \( v \) is preserved in the graph \( \tilde{H} = H \setminus c \) (obtained from \( \tilde{H} \) by removing the vertex \( c \in \mathcal{V} \)) if and only if \( c \) is a walk singlet in \( \tilde{H} \) relative to \( u, v \).

**Proof.** We start with part (i) of the theorem. If \( \mathcal{M}^p_{\gamma} \) is a walk multiplet, then cospectrality of \( \{u, v\} \) is preserved by Theorem 1. For the converse, we assume that \( \{u, v\} \) remain cospectral, that is

\[
[H^k]_{u,u} = [H^k]_{v,v} \quad \forall k \in \mathbb{N},
\]  

(A.26)

where, with \( \tilde{B}_{s,\mathcal{M}}^{(\ell)} \) defined as in Eq. (A.1),

\[
[H^k]_{s,s} = [\tilde{H}^k]_{s,s} + \sum_n \sum_{\ell,\ell'} \sum_{m,m'} [\tilde{H}^l]_{s,m} \gamma_m [H^n]_{c,c} \gamma_{m'} [\tilde{H}^l]_{m',s}
\]  

(A.27)

\[
= [\tilde{H}^k]_{s,s} + \sum_n \sum_{\ell,\ell'} \tilde{B}_{s,\mathcal{M}}^{(\ell)} [H^n]_{c,c} \tilde{B}_{s,\mathcal{M}}^{(\ell)}
\]  

(A.28)

with \( s \in \{u, v\}, \ell, \ell' \geq 0, n \geq 0, \) and \( \ell + \ell' = k - n - 2 \). We further define

\[
A_{\ell,\ell'} \equiv \tilde{B}_{u,\mathcal{M}}^{(\ell)} \tilde{B}_{u,\mathcal{M}}^{(\ell)} - \tilde{B}_{v,\mathcal{M}}^{(\ell)} \tilde{B}_{v,\mathcal{M}}^{(\ell)} = A_{\ell,\ell}, \quad a_n^{(k)} \equiv \sum_{\ell,\ell' = k - n - 2} A_{\ell,\ell'}
\]  

(A.29)

Using \([\tilde{H}^k]_{u,u} = [\tilde{H}^k]_{v,v}\) and substituting the decomposition from Eq. (A.28) into Eq. (A.26) for \( s = u, v \) we arrive at

\[
[H^k]_{u,u} - [H^k]_{v,v} = \sum_{n=0}^{k-2} a_n^{(k)} [H^n]_{c,c} = 0 \quad \forall k \in \mathbb{N}.
\]  

(A.30)

To prove that \( \mathcal{M}^p_{\gamma} \) is a multiplet, we must show that (dropping the subscript \( \mathcal{M} \))

\[
\tilde{B}_u^{(\ell)} = p \tilde{B}_v^{(\ell)} \quad \forall \ell \in \mathbb{N}, \quad p \in \{+1, -1\}.
\]  

(A.31)
We prove this by induction. For \( k = 2 \) (that is, \( n = 0, \ell = \ell' = 0 \)), Eq. \((A.30)\) yields \( [\hat{B}^{(0)}_{u}]^2 = [\hat{B}^{(0)}_{u}]^2 \) or
\[
\hat{B}^{(0)}_{u} = p \hat{B}^{(0)}_{v},
\]
so that Eq. \((A.31)\) is fulfilled in zeroth order \( \ell = 0 \). For the induction step, we assume that Eq. \((A.31)\) is fulfilled up to some arbitrary order \( r \), that is,
\[
\hat{B}^{(\ell)}_{u} = p \hat{B}^{(\ell)}_{v}, \quad \forall \ell < r,
\]
and show that this equation also holds for \( \ell = r + 1 \). To this end, we evaluate Eq. \((A.30)\) for \( k = r + 3 \). For this choice of \( k \), all but two summands vanish, since the assumption Eq. \((A.33)\) implies that \( A_{\ell,\ell'} = 0 \) if \( \ell, \ell' \leq r \). We thus obtain \( A_{1, r+1} + A_{r+1, 1} = 0 \), and since \( A_{1, r+1} = A_{r+1, 1} \), it follows that \( \hat{B}^{(r+1)}_{u} \hat{B}^{(r+1)}_{u} = \hat{B}^{(r+1)}_{v} \hat{B}^{(r+1)}_{v} \). Thus, if \( \hat{B}^{(0)}_{u} \neq 0 \), due to Eq. \((A.32)\) we get \( \hat{B}^{(r+1)}_{u} = p \hat{B}^{(r+1)}_{v} \), as desired.

If \( \hat{B}^{(0)}_{u} = 0 \), it follows from Eq. \((A.32)\) that also \( \hat{B}^{(0)}_{v} = 0 \), and from Eq. \((A.29)\) we obtain \( A_{0,0} = 0 \) for all \( l \). We exploit this fact by evaluating Eq. \((A.30)\) for \( k = r + 4 \), yielding \( A_{1, r+1} = A_{r+1, 1} = 0 \). Now, if \( \hat{B}^{(1)}_{u} = 0 \) we again get \( \hat{B}^{(r+1)}_{u} = p \hat{B}^{(r+1)}_{v} \), as desired. If \( \hat{B}^{(1)}_{u} = 0 \), we proceed to the next higher order \( k = r + 5 \), and so on. In the limiting case where \( \hat{B}^{(\ell)}_{u} = 0 \) \( \forall \ell \leq r \), we evaluate Eq. \((A.30)\) for \( k = 2(r + 2) \), which yields \( A_{r+1, r+1} = 0 \) and therefore \( \hat{B}^{(r+1)}_{u} = p \hat{B}^{(r+1)}_{v} \). This completes the proof of the first part.

For part (ii), we first prove that, if \( c \) is a singlet in \( \tilde{H} \), then its removal does not break the cospectrality of \( u \) and \( v \). To this end, we use the fact that
\[
[\hat{H}^k]_{u,u} = [\hat{H}^k]_{u,u} + \sum_{\ell+n=k} [\hat{H}^\ell]_{u,c} [\hat{H}^n]_{c,u},
\]
and
\[
[\hat{H}^k]_{v,v} = [\hat{H}^k]_{v,v} + \sum_{\ell+n=k} [\hat{H}^\ell]_{v,c} [\hat{H}^n]_{c,v}.
\]
Since \( u \) and \( v \) are cospectral in \( \tilde{H} \), it follows that \( [\hat{H}^k]_{u,u} = [\hat{H}^k]_{v,v} \) for all \( k \), so that \( u, v \) are also cospectral in \( \tilde{H} \) if \( c \) is a singlet in \( \tilde{H} \). For the reverse direction we need to prove that, if the cospectrality of \( u \) and \( v \) is preserved by the removal of a single vertex \( c \), then this vertex must be a walk singlet. With \( \tilde{H} \) being a cone of \( H \) with tip \( c \), and demanding \( u, v \) to be cospectral in both \( \tilde{H} \) and \( H \), combining part (i) of this theorem with Theorem 1 immediately gives that \( c \) must be a singlet in \( H \).

\[ \square \]

**Theorem 4 (Eigenvector components on walk multiplets).** Let \( H = H^T \in \mathbb{R}^{N \times N} \) represent a graph with a pair of cospectral vertices \( u, v \), and let its eigenvectors be chosen according to Lemma 1. Then any eigenvector \( \phi \) of \( H \) with eigenvalue \( \lambda \) and nonzero components of odd (even) parity \( p \) on \( u, v \),
\[
\phi_u = p \phi_v \neq 0, \quad p \in \{+1, -1\},
\]
fulfills
\[
\sum_{m \in \mathbb{M}} \gamma_m \phi_m = 0
\]
if and only if \( \mathbb{M}^{\gamma_p} \) is a walk multiplet relative to \( u, v \) with even (odd) parity \( -p \) and weight tuple \( \gamma = (\gamma_m)_{m \in \mathbb{M}} \).

**Proof.** Using the spectral decomposition
\[
H = \sum_{\nu=1}^{N} \lambda_{\nu} \phi_{\nu}^T \phi_{\nu}^T
\]
of $H$ in the orthonormal eigenbasis $\{\phi^\nu\}$, chosen according to Lemma 1, we have, for $s \in \{u, v\}$,

$$[H^k]_{v,m} = \sum_{\nu=1}^{N} \lambda^k_{\nu} \phi^\nu u \phi^\nu_{m} = \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu u \phi^\nu_{m} + \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu s \phi^\nu_{m} \quad \forall k \in \mathbb{N}, \tag{A.39}$$

where we have collected the labels $\nu$ of eigenvectors with parity $\pm 1$ on $\{u, v\}$ into the set $\mathbb{N}^\pm$ (the remaining eigenvectors with $\phi^\nu_u = \phi^\nu_v = 0$ do not appear in the sum). Note that Eq. (A.39) incorporates the spectral decomposition of the identity matrix, $I_{s,m} = \sum_{\nu=1}^{N} \phi^\nu u \phi^\nu_{m}$ for $k = 0$, meaning that $\lambda^0_{\nu} = 1$ even in the case of zero eigenvalues. Next we calculate:

$$[H^k]_{v,m} - p[H^k]_{v,m} = (1 - p) \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu u \phi^\nu_{m} + (1 + p) \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu s \phi^\nu_{m} \tag{A.40}$$

$$= 2 \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu u \phi^\nu_{m}, \tag{A.41}$$

where we used the parity of eigenstates on $\{u, v\}$, i.e. $\phi^\nu u = \pm \phi^\nu v$ for $\nu \in \mathbb{N}^\pm$, so that the sum over $\nu \in \mathbb{N}^\pm$ vanishes for $p = \pm 1$. Multiplying by $\gamma_{m}$ and summing over $m \in \mathbb{M}$ we obtain

$$B_{u;m}^{(k)} - p B_{v;m}^{(k)} = 2 \sum_{\nu \in \mathbb{N}^+} \lambda^k_{\nu} \phi^\nu u \sum_{m \in \mathbb{M}} \gamma_{m} \phi^\nu_{m}, \tag{A.42}$$

with $B_{u;m}^{(k)}$ defined as in Eq. (A.1). It follows that, if Eq. (15) is fulfilled with $\phi = \phi^\nu$, for all $\nu \in \mathbb{N}^\pm$, then $B_{u;m}^{(k)} = p B_{v;m}^{(k)} \forall k$ and thus $M^p$ is a walk multiplet relative to $\{u, v\}$ with parity $p$. Conversely, if $M^p$ is a multiplet, then the left side of Eq. (A.42) vanishes $\forall k \in \mathbb{N}$. For $k \in [0, n_p - 1]$, where $n_p \equiv |\mathbb{N}^\pm|$, we can write Eq. (A.42) in the matrix form

$$Vc = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \lambda^1_{\nu} & \lambda^2_{\nu} & \cdots & \lambda_{n_p}^\nu \\ \vdots & \vdots & \ddots & \vdots \\ \lambda^{n_p-1}_{\nu} & \lambda^1_{\nu} & \cdots & \lambda_{n_p-1}^\nu \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n_p} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \tag{A.43}$$

with coefficients $c_{\nu} = 2 \phi^\nu u \sum_{m \in \mathbb{M}} \gamma_{m} \phi^\nu_{m}$, where $V^T$ is the (square) Vandermonde matrix with $[V^T]_{i,j} = \lambda^i_{\nu} = x_{\nu}^{-1}$, yielding

$$\det(V) = \det(V^T) = \prod_{1 \leq \nu \leq n_p} (\lambda_{\nu} - \lambda_{\nu}). \tag{A.44}$$

Now, our choice of eigenvectors ensures that $\lambda_{\nu} \neq \lambda_{\nu} \forall \nu \neq \mu$ with $\nu, \mu \in \mathbb{N}^\pm$, so that $\det(V) = 0$. Thus $V$ is invertible, so that Eq. (A.44) yields $c_{\nu} = 0 \forall \nu \in \mathbb{N}^\pm$, and since $\phi^\nu_u \neq 0$ we have that $\sum_{m \in \mathbb{M}} \gamma_{m} \phi^\nu_{m} = 0 \forall \nu \in \mathbb{N}^\pm$, completing the proof.

\[\square\]

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