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# Structural covariance of graphs

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Algebraic structures including multiple rank tensors, linear and non-linear operators are related to and represented with various types of graphs. Special emphasis is placed on linear operators e.g. on the Hilbert space. A different graph represents the same operator depending on the basis frame used, in general non-orthonormal. All such graphs are shown to belong in one equivalence class and are termed "structurally covariant". Crucial indices related to eigenvalues but invariant under any basis frame changes including non-orthonormal ones provide one way to characterize each class. A set of rules are given that allow one to find the graphs structurally covarinat with a given one and/or to deduce the class indices directly by simple pictorial manipulations on a graph. Applications in various fields including the quantum theory of molecules and reactions are indicated.

**Key words:** Structural covariance—transformation of graphs

## 1. Introduction

A graph is a superposition out of a set of dots (vertices) and lines.[1] The lines may have scalar "strengths" associated with them. If the lines have direction we have the "diagraph" [2].

Graphs have been useful in problems involving counting [3, 4], coloring [1], transversing [1, 3], and in many applied fields [2, 4]. A sizable gap remains however between graphs, and the subject of algebraic topology [5, 6] with its more powerful theorems.

The usefulness of graphs is considerably extended if they are associated with some algebraic structures as in the theory presented below. The notions introduced, in particular the "structural covariance" of graphs will relate seemingly

unrelated graphs to each other, classify them into certain equivalence classes providing thereby some rather useful tools for quantum theory, for the electronic structure theory of molecules, for the dynamics of coupled systems, some linear, some non-linear, as in chemical reaction systems.

Discrete, rigid, hence geometric objects in Euclidean $n$-space, or for example in the finite dimensional subspaces of the Hilbert space, have symmetries and invariance properties [7] under some subgroups of the $O(n)$ or $U(n)$, (the orthogonal or unitary groups) [8] or under the $O(n)$ or $U(n)$ themselves [7]. In "structural covariance", graphs built on $n$-spaces need not have symmetries, but more generally transform into each other if in the same "$L$-class", this following as will be shown below, from the principle of linear covariance introduced earlier [9].

In what follows, we first relate and represent algebraic structures with graphs, then derive some simple-to-use rules that allow one to find the graphs structurally covariant with a given one. One then determines also the crucial invariants of such a class of graphs, invariants more general than those of spatial or Hilbert space symmetries. Some applications for chemical physics and dynamics are noted, these forming the subjects of additional publications.

## 2. Algebraic structures and their graphs

Let $\{|e_i)\}$ be a basis, orthonormal (O.N.) or non-O.N., for $V_n$, a linear vector space of dim $V_n = n$. We shall take $V_n$ in this paper over the real field $R$, i.e. $V_n \equiv V_{n,R}$ which cover most of the applications. Extension to the complex field which allows several more results especially for quantum theory is deferred.

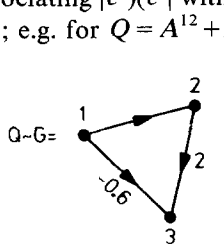
To each $|e_i)$ we associate a *dot* (a vertex). [More precisely an "out-vertex", $\bullet\triangleright$ to $|e_i)$, and an "in-vertex" $\triangleright\bullet$ to $(e_i|$ the adjoint (or to $(e^i|$, the contravariant and adjoint, if the basis is non-O.N.) [9]].

A linear operator on $V_n$, e.g. $Q$ is an $n^2$-term dyad over $R$.

$$Q = q_{ij}|e^i)(e^j|; \qquad q_{ij} \in R \tag{1}$$

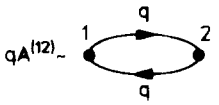
Such operators are written as "*L-invariants*", i.e. independent of any linear basis-"frame" [9], with $\{q_{ij}\}$ transforming covariantly while $\{A^{ij} \equiv |e^i)(e^j|\}$ contravariantly under any $S \in L(n, R)$, the linear group ($\equiv$"$L$").

Associating $|e^i)(e^j|$ with a *directed line* from $i$ to $j$, a $Q$ gets denoted by a digraph, $G_D$; e.g. for $Q = A^{12} + 2A^{23} - 0.6A^{13}$,




(2)

If $Q$ is a self-adjoint operator, then for each $(i, j)$, there is in $Q$ a symmetric combination $A^{(ij)} \equiv |e^i)(e^j| + |e^j)(e^i|$




(3a)

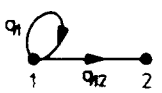
For such $Q$, we shall replace Eq. (3a) with an (undirected) line:


(3b)

Thus Hermitian $Q$ have undirected graphs, $G$. If no "strength" $q$ is indicated on a line of $G$, it is implied that $q = +1$.

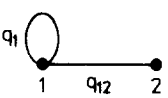
$Q$ may contain diagonal dyads, $A^i \equiv |e^i)(e^i|$ (no sum) which introduce loops [10, 11] in $G_D$ or $G$; e.g.

$$Q = q_1|e^1)(e^1| + q_{12}|e^1)(e^2| \sim$$

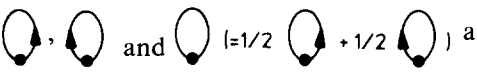



(4a)

$$Q' \equiv q_1|e^1)(e^1| + q_{12}A^{(12)} \sim$$




(4b)

Since a directed loop can be twisted, 

are equivalent.

Various other algebraic structures [12] on $V_n$ can be generated as higher rank tensors $\left\{ T \begin{matrix} rx|), sx(| \\ px|), qx(1 \end{matrix} \right\}$ with $p, q, r, s$, integers. The $T$ are tensors under $L(n, R)$.

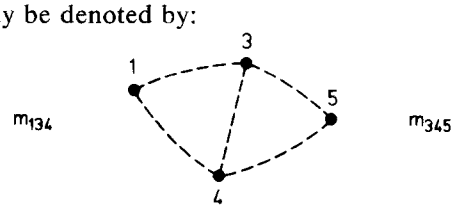
While linear operators on $V_n$ are covered by $\{T^{|}_{|}, T_{|)(|}$, or $T^{|)(|}\}$, higher rank tensors are needed for many-particle problems [13], in second quantization, and in some non-linear problems such as non-linear chemical kinetics and ecological dynamics.

While 1,1-tensors go into graphs similar to those in customary graph theory [1, 2], algebraic structures of higher rank mixed tensors required graphs with several kinds of lines [11, 14].

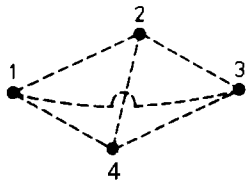
$N$-particle states in quantum theory, for example $|\Psi\rangle$ of $N = 3$,

$$|\bar{\Psi}\rangle = m_{ijk}|e^i)|e^j)|e^k) \tag{5}$$

use $T^{3x|)}$, two superimposed terms of which, e.g. $[m_{134}|e^1)|e^3)|e^4) + m_{345}|e^3)|e^4)|e^5)]$ may be denoted by:



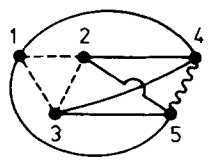
(ignoring arrows), while a fourth rank tensor's term $|e_1)|e_2)|e_3)|e_4)$ would look like




a *complete graph* [3], the $K_4$. Thus a $|\Psi\rangle$ for a given $N$, will be a weighted superposition of several $K_n$.

With the simplest mixed tensor, (1,1), in the $G$, a loop corresponds to a projection operator, a line $(ij)$ to a "shift operator" from $|e_j)$ to $|e_i)$ or a 2-permutation.

For higher mixed tensors then (1,1), three kinds of lines are needed. E.g. for the $|e_1)|e_2)|e_3)(e^4|(e^5|$ component




The product of $N$-kets forms a $K_N$, the product of $M$-bras another complete subgraph $K_M^+$, while the two sets of vertices are fully connected from one set to the other constituting $K_{N,M}$, a complete *bipartite graph* [1, 3].

The graph of a covariant $N$th rank tensor (kets product) is *planar* [1, 3, 11] for $N \leq ,4$, *non-planar* for $N \geq 5$. Similarly for the contravariant $N$-dyad (bras). The graph of an $N \times M$ mixed tensor is planar for $N, M < 3$, non-planar for $N, M \geq 3$, these by the Kuratowski theorems [3]. Beyond that the 1- and 2-topologies may be developed as in Ref. [11].

Although such graphs appear complicated, they can be studied by compressing the $K_N$ into a "super-dot" of weight related to $N$, or of $N$, and $K_M^+$ into another one of $(M)$. (cf. Ref. [11]).

The rest of this paper will concentrate on the 1,1-tensors and linear operators on $V_n$ itself which make a convenient connection to ordinary graphs with more general results than possible with the usual matrix identifications [14].

### 3. Graphs representing the same operator on different basis frames

An abstract linear operator $Q$ on $V_n$ is a $L(n, R)$-frame invariant [9]. On a particular $L$-basis frame, O.N. or non-O.N., $\{|e_i)\}$ with $(e_i|e^j) = \delta_i^j$, but in general $(e_i|e_j) = \Delta_{ij} \neq \delta_{ij}$; $(|\Delta| \neq 0)$, the $Q$ is represented by $Q = IQI \Rightarrow$ Eq. (1). Assuming $Q = Q^+$ (self-adjoint), $Q = q_{ij}A^{(ij)}$. Where $q_{ij} \neq 0$, there will be an $ij$-line in the graph of $Q$.

Though $Q$ is $L$-invariant, the graph $G$ of $Q$ is $L$-frame dependent. *All* $\{G, G', G'', \ldots\}$ obtained by transforming the initial $L$-frame by an $S \in L(n, R)$

will be termed "structurally covariant". All such $\{G\}$ belong in one and only one $L$-equivalence class [15]. The question is however how to generate such graphs from a known one by simple manipulations on a graph itself (Sect. 4).

## 4. Graphs of different operators on the same $V_n$

Let $Q$ and $P$ be two linear operators on $V_n$ each written out on a different $L$-frame thereby having the graphs $G_Q$ and $G'_P$. In general $G_Q \neq G'_P$, as also on the same frame $G_Q \neq G_P$.

If there exists an $L$-frame such that on it $\bar{G}_Q$ looks the same as a $\bar{\bar{G}}_P$ in some (in general other) $L$-frame, then we say $Q \overset{L}{=} P$ or $Q \overset{sc}{=} P$, i.e. $Q$, $P$ are in the same equivalence class. (*Proof*: $\bar{G}_Q \overset{L}{=} Q$, $\bar{\bar{G}}_P \overset{L}{=} P$; $\bar{G}_Q = \bar{\bar{G}}_P$; $\therefore Q \overset{L}{=} P$). Then, and only then, the $\{n_+, n_0, n_-\}$, $n = n_+ + n_0 + n_-$, the number of $(+)$, zero, and $(-)$ eigenvalues of $Q$ and $P$ will be the same, and conversely.

Other, covariant, contravariant, and higher rank mixed tensors and operators, too, are classified under $L(n, R)$ acting on $V_n \times V_n \cdots \times V_n^+ \times \cdots V_n^+$ into $L$-equivalence classes.

## 5. Graphs of operators on different vector spaces $V_n(\boldsymbol{R})$ of a vector space field

In some problems, particularly the quantum theory of molecules, there is a different $V_n(\boldsymbol{R}_{3n})$ at each point $\boldsymbol{R}_{3n}$ of an Euclidean $3n$-space $\mathscr{E}_{3n}$ corresponding e.g. to a spatial configuration of a molecule in $\mathscr{E}_3$. These $\{V_n(\boldsymbol{R})\}$ define [16] a vector space field with each $V_n(\boldsymbol{R})$ isomorphic to a standardized $V_n$ which is independent of $R$.

Let $Q(\boldsymbol{R})$ and $P(\boldsymbol{R}')$ be operators on $V_n(\boldsymbol{R})$ and $V_n(\boldsymbol{R}')$ respectively. If in some $L$-frame in $V_n(\boldsymbol{R})$, $G_Q$ looks the same as a $G_P$ of $P$ on some $L$-frame in $V_n(\boldsymbol{R}')$, then $Q$ and $P$ will be said to be structurally covariant ($Q \overset{sc}{=} P$). (Proof follows from mapping $V_n(\boldsymbol{R})$ and $V_n(\boldsymbol{R}')$, then $Q$ and $P$ onto the std. $V_n$ and $V_n \times V_n^+$, then Sect. 4).

## 6. Rules for generating structurally covariant graphs

On any $L$-frame, in general non-O.N., in a $V_n$, an operator $Q$ is given by Eq. (1). A linear transformation $S \in L(n, R)$, hence $|S| \neq 0$, takes one to another $L$-frame.

$$S: \{|e_i)\} \to \{|f_k)\} \tag{6a}$$

$$Q = q^{ij} A_{(ij)} = \bar{q}^{kl} B_{(kl)}$$

$$(B_{(kl)} \equiv |f_k)(f_l| + |f_l)(f_k|).$$

$$Q = (S^{k\cdot}_{\cdot i} q^{ij} S^{\cdot l}_{j})(S^{\cdot r}_{k} A_{(rs)} S^{s}_{\cdot l}). \tag{6b}$$

Any $S$ in Eq. (6a) basically gives a linear combination of $\{|e_i)\}$ over $R$. It therefore can be constructed from a succession of $(a)$ multiplication of an $|e_i)$ by a scalar $\alpha(\neq 0) \in R$, $(b)$ addition of an $|e_i)$ to an $|e_j)$, and $(c)$ permutation of a pair $(i, j)$.

The corresponding contravariant transforms ($a'$) division by $\alpha$, ($b'$) subtraction of ($i$) from ($j$), and ($c'$) re-permutation of ($i, j$), are applied in reverse order [$S^{-1}$].

The $L$-transform of $A_{(ij)}$ from

$$S: \{|e_i)(e_j| + |e_j)(e_i|\} \to \{|f_k)(f_l| + |f_l)(f_k|\} \tag{7a}$$

i.e.

$$S: \{A_{(ij)}\} \to S\{A_{(ij)}\}S^+ \tag{7b}$$

$S$ preserves the symmetric property, ($ij$).

$S \in L(n, R)$ may be applied to the object $Q$ itself, changing it into *another* operator $\bar{Q}$ in $V_n \times V_n^+$.

$$S: Q \to \bar{Q}. \tag{8}$$

This actual change, as contrasted to an $L$-frame transform which kept $Q$ the same in Eq. (6b), is carried out either by $SAS^+$ alone, or by $(S^{-1})_q^+(S^{-1})$ alone, but not both.

The $\{Q, \bar{Q}, \dots\}$ related by Eq. (8) are on the same "$L$-orbit", they are in the same $L$-equivalence class [15], ($Q \overset{L}{=} \bar{Q} \overset{L}{=} \bar{\bar{Q}} \cdots$).

Thus a set of graphs $\{G\}$ on $V_n$, may represent *i*) a set of distinct linear operators $\{Q\}$, and/or *ii*) representations on O.N. or *non*-O.N. basis frames of the same $Q$. Either case, all $G$'s on $V_n$ are classified into $L$-equivalence classes. Each graph belongs in one and only one $L$-class. Those $\{G\}$ of the same $L$-class are "structurally covariant".

The elementary operations that constitute any $S \in L(n, R)$ in the ket-bra algebra are quite straightforward. The corresponding graph operations on $\{G\}$ however are not known. They are given below for undirected graphs which represent Hermitian operators. The rules for directed graphs have different applications and will be presented elsewhere.

**Rule – S1:** Any vertex of a $G$ can be multiplied by an arbitrary scalar $\kappa \in R$, positive or negative, but not zero, without changing the $L$-class of $G$. ($G \overset{sc}{=} G'$).

Multiplication of a vertex $i$ by $\kappa$ means all lines (or their strengths) coming out (undirected) of that $i$ are multiplied by $\kappa$. A loop at $i$ is however multiplied by ($\kappa^2$).

*Proof*: In

$$Q = q^{ij}|e_i)(e_j| \sim G$$

taking e.g. the $i = 1$ vertex, the sum over the other index $j$ gives the "star" of 1, i.e. all the lines of 1.

$$Q = \sum_{j>1}^{n} q^{1j}|e_1)(e_j| + \sum_{i>1}^{N} q^{i1}|e_i)(e_1| + q^{11}|e_1)(e_1| \tag{9}$$

Multiplying the vertex 1 implies $|e_1) \to \kappa|e_1)$ *and* $(e_1| \to \kappa((e_1|$ yielding in $Q$ therefore $\sum_{j\neq 1} \kappa q^{1j}|e_1)(e_j|$, the $\kappa$-stretched out-going lines from (1), *and*

$\sum_{i\neq 1} \kappa q^{i1}|e_i)(e_1|$, $\kappa$-stretched incoming lines to 1. Hence the undirected lines are $\kappa$-stretched. The loop becomes $\kappa|e_1)(e_1|\kappa = \kappa^2|e_1)(e_1|$.

The $\kappa$-multiplication is an $SQS^+ = Q'$ form with this $S(\kappa) \in L(n, R)$. Thus $Q \overset{L}{=} Q'$.

**Rule – S2:** Any vertex (i) without loops can be lifted up and placed onto any other vertex $(j)$ not directly connected to $(i)$ carrying the lines of $(i)$ onto $(j)$. The original lines are also retained. If in the process two lines superimpose their strengths are algebraically added.

*Proof*: The operation is $|e_i) \to |e_i) + |e_j)$ and simultaneously on the bra. This is an elementary $S \in L(n, R)$ and $S^+$ for the bra. On a $Q = Q^+$, therefore $Q \overset{sc}{=} \bar{Q}$ and $G \overset{sc}{=} \bar{G}$.

For the $(i)$ terms of $Q$, i.e. the "star" of $(i)$ in $G(\equiv i^*)$

$$i^* \equiv \sum_{k\neq i} q^{ik}[|e_i)(e_k| + |e_k)(e_i|]$$

$$\to i^* + \sum_{k\neq j} q^{ik}[|e_j)(e_k| + |e_k)(e_j|]$$

Thus $G$ acquires additional lines from $j$ to the original star-termini of $i$. The degree of $j$ is increased. The new $\bar{G}$ is structurally covariant with $G$.

**Rule – L1:** If $i$ and $j \in G$ are directly connected ($q^{ij} \neq 0$), when the star of $i$ is placed on $j$ as in *Rule – S2*, $j$ acquires in addition a loop of strength $2q^{ij}$.

*Proof*: When $|e_i) \to |e_i) + (e_j)$ (and the bras) in $Q$, the term $q^{ij}[|e_i)(e_j| + |e_j)(e_i|]$ gets added the term $2q^{ij}|e_j)(e_j|$.

**Rule – L2:** If $(i)$ had a loop on it of strength $q^{ii}$, when the star of $i$ is added onto $(j)$, a line $(ij)$ of strength $q^{ii}$ is added from $i$ to $j$ (undirected here for $Q = Q^+$) as well as a loop of strength $q^{ii}$ shows up of $(j)$. The original loops and lines in $G$ are too retained. Then $\bar{G} \overset{sc}{=} G$.

*Proof*: With $|e_i) \to |e_i) + |e_j)$, and similarly for $(e_i|$, $q^{ii}|e_i)(e_i| \to q^{ii}|e_i)(\bar{e}_i + q^{ii}[|e_i)(e_j| + |e_j)(e_i|] + q^{ii}|e_j)(e_j|$.

In addition to the linear combination operations generated by the four rules above, an $S \in L(n, R)$ may also contain some permutations, e.g. $|e_i) \to |e_j)$, and $|e_j) \to |e_i)$. Permutations simply permute the vertex labels on a $G$. These would affect sometimes a rigid geometry, but do not alter the nature of $G$ as a graph (or a simplicial complex).

The above, two star-rules, and two loop rules may be applied any number of times and in any sequence desired, to a $G$. Any $SQS^+ = \bar{Q}$ hence $Q \overset{sc}{=} \bar{Q}$ can be carried out this way on a $G$ of $Q$. Any $S \in L(n, R)$ can be constructed this way, including some permuations. Conversely any star-loop operations combination is an $S \in L(n, R)$.

The following lemma may also be found at times useful vis-a-vis operations on a $G$. *Lemma*: If $G = G_1 \oplus G_2 \oplus \cdots$, a superposition of not necessarily connected subgraphs, star-loop operations (and permutations) may be applied simultaneously to each subgraph; then $\bar{G} = \bar{G}_1 \oplus \bar{G}_2^+$. (Proof is immediate from the bilinearity of $Q$ and the linearity of $S$).

## 7. Two kinds of uses of the rules and examples

Given a linear operator $Q$ on $V_{n,R}$ or a graph $G$ representing such a self-adjoint $Q$ on some linear basis frame, O.N. or non-O.N., the rules may be used in two ways: (*i*) to deduce directly from a $G$ of $Q$, the crucial $L(n, R)$ invariants, i.e. the LPI $\equiv \{n_+, n_0, n_-\}$, the numbers of (+), (0), and (−), eigenvalues of $Q$ (and of the entire $L$-class $\supset \{G_Q\}$). In e.g. electronic structure theory, the LPI are physically the most crucial properties, the numbers of bonding, non-bonding, and anti-bonding molecular orbitals of $Q \to h$, the Hückel-like MO Hamiltonian.

(*ii*) Various $Q$'s or $G$'s structurally covariant with the given ones, therefore in the same $L$-class, and hence with the same LPI may be deduced by simple pictorial manipulations on a $G$ only. In molecular theory, this gives the set of molecules or atom clusters which have qualitatively the same "thermicity" or rough stability. One sees that two different looking molecules if structurally covariant, in fact *look the same* (same $G$) after describing one in a certain new linear "coordinate" (basis) frame which is in general non-orthonormal (hence overlooked in quantum chemistry hitherto) [15].

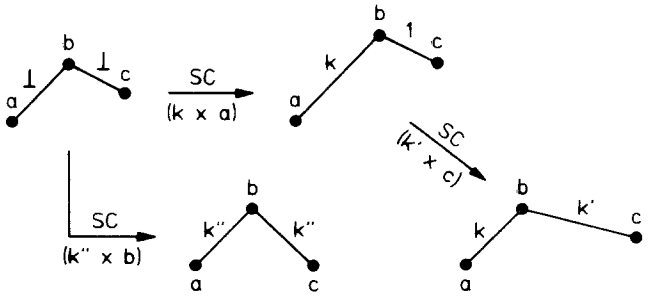
Since the LPI are also directly related to the *rank* $(n - n_0)$, and *signature* $(n_+ - n_-)$ of $Q$, the rules also readily give these from any $G$ description of a $Q$. Many applications in mathematical physics require these quantities.

One significant use of the rules, would be also in seeing which parameter changes in a $Q$ would affect the LPI and which not, thereby charting out the physical or computational regions for $\{Q\}$ with the same qualitative behavior.

In another set of applications, in network dynamics [16] and dynamic stability theory [17], a local $Q$ around a steady state is in general non-Hermitian. Then the version of the present rules for directed graphs [18] may be used to determine regions of stability, or types of instability around steady states in coupled reaction systems.

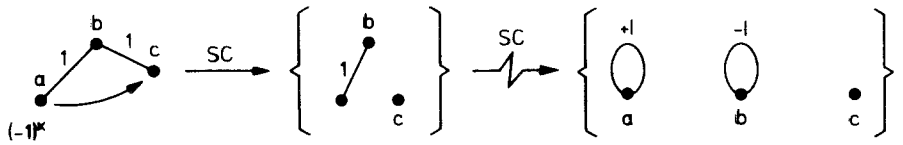
Several examples below for $Q = Q^+$ with undirected $G$'s illustrate the rules and some of their applications.

*Examples*: (A) To illustrate first the star and loop rules as well as give a result interesting in itself, we take any straight or branched chain with lines of strength +1. E.g. for $n = 3$, in Eq. (G1), we see by rule-S1 that multiplying any vertex with an arbitrary number $\kappa$ causing thereby various types of stretches of (abc) leaves the graph structurally covariant and therefore also of the same LPI.




(G1)

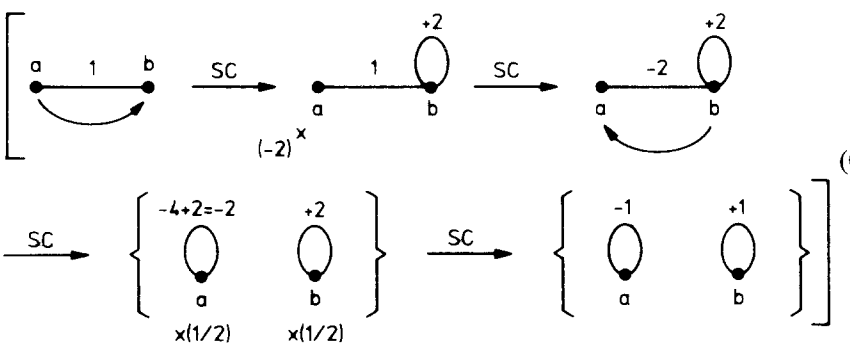
Similarly multiplying say $a$ with $(-1)$, but then by rule-S2, taking $a$ onto $c$ yields in (G2),




(G2)

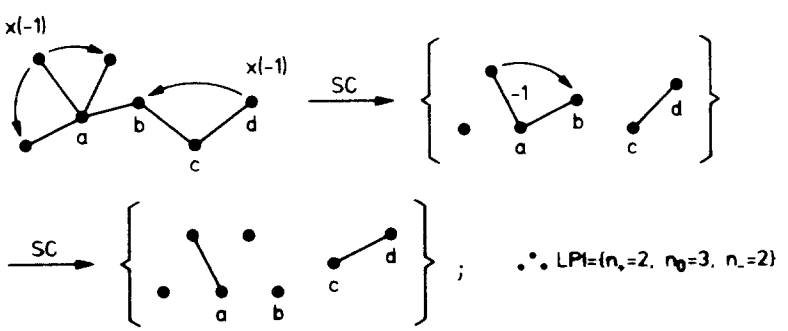
In the last step, a single line segment ($ab$) that results has the sub-LPI, $n_+ = 1$, $n_- = 1$ as can be deduced by the loop rules as in (G3).

The above example gives e.g. the MO level patterns of $H_3$ and $H_3^+$ during various large deformations of these species.




(G3)

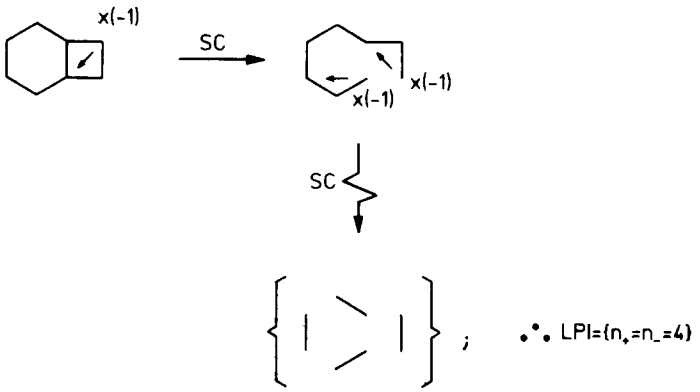
For a branch attached to a "star" type of graph as in (G4):




(G4)

Thus using the rules, theorems for the numbers of (+), (0), and (−) eigenvalues of any size and type of "tree" with even or odd $n$, with any number of straight chain or star subgraphs are readily deduced.

(B) With graphs involving single or multiple rings, our first strategy will be to use the rules so as to break open the rings. Then to find the LPI, the rules are used so as to reduce the graphs into a number of isolated dots ($\# = n_0$), and single line segments ($\# = n_+ = n_-$). Along the way various graphs result each structurally covariant with the initial graph and to each other. E.g.




In such ways, the LPI's and structurally covariant sets of a large number of planar and non-planar graphs (in both the Kuratowski sense and the ordinary sense) and "homologous" series of graphs have been derived by the author and will be reported as a compilation.

The MO level pattern of classes of molecules as well as their behaviour after large deformations or rearrangements are similarly derived.

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