Novel highly symmetrical trivalent graphs which lead to negative curvature carbon and boron nitride chemical structures

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Abstract

A graph described by Klein in the 19th century consisting of 24 heptagons can be used to generate possible but not yet experimentally realized carbon structures through such a leapfrog transformation. The automorphism group of the Klein graph is the simple PSL(2,7) group of order 168, which can be generated from $2 \times 2$ matrices in a seven-element finite field $\mathbb{F}_7$ analogous to the generation of the icosahedral group of order 60 by a similar procedure using $\mathbb{F}_5$. Similarly, a graph described by Walther Dyck, also in the 19th century, consisting of 12 octagons on a genus 3 surface, can generate possible carbon or boron nitride structures consisting of hexagons and octagons through a leapfrog transformation. The automorphism group of the Dyck graph is a solvable group of order 96 but does not contain the octahedral group as a normal subgroup and is not a normal subgroup of the automorphism group of the four-dimensional analogue of the octahedron.

Keywords: Klein graph; Dyck graph; Automorphism groups; Graph spectra

1. Introduction

Many interesting carbon and boron nitride chemical structures can be constructed from polygonal networks of trigonal (sp²-hybridized) atoms and thus can be described by trivalent graphs. The flat graphite and corresponding boron nitride structures arise if all of the polygons are hexagons and correspond to the well-known \{6,3\} tessellation (Fig. 1a). Positive curvature arises if some of the polygons have less than six edges and the resulting structures are closed polyhedral cages. In the most favorable structures no pair of non-hexagons shares any edges. Such structures are said to satisfy the isolated non-hexagon rule (INHR). Of particular interest is the truncated icosahedral structure (Fig. 1b) exhibited by the experimentally observed C₆₀ fullerene, which has 12 pentagonal faces and 20 hexagonal faces [11]. This structure can be generated through such leapfrog transformations.
by a so-called leapfrog transformation of the regular dodecahedron, which consists of omnicapping (stellation) followed by dualization to triple the number of vertices from 20 to 60 (Fig. 2a) [5]. Such leapfrog transformations on trivalent graphs containing polygons other than hexagons triple the number of vertices while preserving the automorphism group of the original graph and provide the minimum number of new hexagons to ‘dilute’ the non-hexagons in the original graph so that the INHR rule is satisfied. A similar leapfrog transformation on the cube (Fig. 2b) generates the truncated
octahedron, which is a promising candidate for a boron nitride structure since it is a bipartite graph which allows construction of a structure having an equal number of boron and nitrogen atoms and only boron–nitrogen chemical bonds (i.e., all edges connect a boron vertex with a nitrogen vertex).

If the only non-hexagons in the INHR carbon or boron nitride structure have more than six edges, then negative curvature structures are required. Favorable structures of this type exhibiting the highest possible symmetries are based on infinite periodic minimal surfaces [1] having genus 3 unit cells, where a unit cell refers to the unit that repeats to form the infinite three-dimensional lattice. A suitable carbon structure containing only hexagons and heptagons with the minimum number of hexagons required to satisfy the INHR can be generated by a leapfrog transformation on a genus 3 surface containing 24 heptagons based on a graph described in the 19th century by Felix Klein [6,8,9]. Similarly, a suitable carbon or boron nitride structure containing only hexagons and octagons with the minimum number of hexagons to satisfy the INHR can be generated by a leapfrog transformation on a genus 3 surface containing 12 octagons described by Walther Dyck in the 19th century [4].

This paper summarizes some of the properties of the Klein and Dyck graphs which can be used to generate possible negative curvature carbon and boron nitride structures through leapfrog transformations.

2. Applications of Euler’s theorem

The only regular trivalent polyhedra are the tetrahedron, cube, and dodecahedron as can be demonstrated readily by the use of Euler’s theorem. The leapfrog transformations on these regular polyhedra triple their numbers of vertices while preserving their automorphism groups to give the truncated tetrahedron, the truncated octahedron, and the truncated icosahedron, respectively. The truncated icosahedron is found in the well-known C60 fullerene [11].

Trivalent regular graphs having a single kind of polygonal face with more than six edges do not correspond to regular polyhedra, but instead correspond to networks embedded on surfaces of non-zero genus [7]. The lowest non-zero genus leading to surfaces that can be embedded symmetrically in three-dimensional space is genus 3. Euler’s theorem can be generalized to trivalent graphs embedded on a surface of genus 3 using the relationship

\[ v - e + f = 2(1 - g), \]

where \( v, e, \) and \( f \) are the numbers of vertices, edges, and faces, respectively, and \( g \) is the genus. Note that for \( g = 0 \) (e.g., for polyhedra homeomorphic to a sphere) this equation reduces to the standard version of Euler’s theorem. Applying Eq. (1) to surfaces of genus 3 gives

\[ v - e + f = -4. \]
Applying this equation to a trivalent graph of genus 3 and using the relationships
\[ 2e = 3v, \]  
\[ \sum_n f_n = f \]  
and
\[ \sum_n n f_n = 2e, \]
where \( f_n \) denotes the number of \( n \)-gon faces, leads to
\[ \sum (6 - k) f_k = -24. \]  
Setting \( f_7 = 0 \) gives \( f_7 = 24 \) corresponding to the Klein graph (Fig. 3a) [8,9] whereas setting \( f_8 = 0 \) gives \( f_8 = 12 \) corresponding to the Dyck graph (Fig. 3b) [4]. Application of the above equations shows that the Klein graph has 56 vertices, 84 edges and 24
heptagonal faces whereas the Dyck graph has 32 vertices, 48 edges, and 12 octagonal faces. The duals of these graphs can be generated in the standard way by exchanging face midpoints and vertices.

3. The Klein graph

3.1. The automorphism group of the Klein graph

The automorphism group of the Klein graph (Fig. 3a) bears an interesting relationship to that of the regular icosahedron if these groups are defined using $2 \times 2$ matrices with the entries in finite fields of $p$ elements where $p$ is a prime [10]. In this connection the group SL(2, $p$) is defined to be the group of all $2 \times 2$ matrices having determinant 1 with entries in the finite field $\mathbb{F}_p$. Its subgroup PSL(2, $p$) for odd $p$ is defined to be the quotient group of SL(2, $p$) modulo its center. The group PSL(2, 5), defined in this manner, contains 60 elements and is isomorphic to the icosahedral pure rotation group $I$ or the alternating group $A_5$ with the following conjugacy class structure $E + 12C_3 + 12C_5 + 20C_3 + 15C_2$, where $C_n$ refers to an operation of period $n$ and $E$ is the identity operation. Analogously, the group PSL(2, 7) contains 168 elements and is the automorphism group of the Klein graph with the conjugacy class structure $E + 24C_7 + 24C_7^3 + 56C_3 + 21C_2 + 42C_4$. An important property of the PSL(2, $p$) groups for the three primes 5, 7, and 11, but for no other primes is that they can function as transitive permutation groups on sets of either $p$ or $p + 1$ objects [10]. The PSL(2, $p$) groups ($p$=5, 7, and 11) are all simple groups but have the tetrahedral, octahedral, and icosahedral groups as subgroups. Because of this subgroup structure the PSL(2, $p$) groups for $p$=5, 7, and 11 have been called the pentakistetrahedral, the heptakisoctahedral, and the undecakiscicosahedral groups, respectively [3].

3.2. The spectra of the Klein graph and its dual

The spectra of the Klein graph (Fig. 4) and its dual (Fig. 5b) have been determined using Mathematica [3]. The spectrum of the Klein graph dual (Fig. 5b) bears an interesting resemblance to that of the icosahedron (Fig. 5a) with the required non-degenerate 3 eigenvalue, a $p$-fold degenerate −1 eigenvalue ($p$=5 for the icosahedron and 7 for the Klein graph dual), and matching degenerate $\pm \sqrt{p}$ eigenvalues ($p$=5 for the icosahedron and 7 for the Klein graph dual).

4. The Dyck graph

4.1. The automorphism group of the Dyck graph

The automorphism group of the Dyck graph (Fig. 3b) has 96 elements with the conjugacy class structure $E + 24S_8 + 6C_4 + 3C_4^2 + 32C_3 + 12C_2 + 18S_4$ where $C_n$ and
Sn both refer to operations of period n with different numbers of fixed points. This group, is a solvable group with the following normal subgroup chain using Dyck’s nomenclature [4] for the larger groups in the chain:

\[ G[2, 3, 8] \rightarrow G[3, 3, 4] \rightarrow G[4, 4, 4] \rightarrow D_{2h} \rightarrow D_2 \rightarrow C_2 \rightarrow C_1 \]

Order : 96 48 16 8 4 2 1

The octahedral group is not a normal subgroup of \( G[2, 3, 8] \) nor is the group \( G[2, 3, 8] \) a normal subgroup of the automorphism group of the four-dimensional analogue of the octahedron [2] as can be determined by comparison of the conjugacy classes.

4.2. The spectra of the Dyck graph and its dual

The spectra of the Dyck graph (Fig. 6a) and its dual (Fig. 6b) have been determined using Mathematica. These spectra are seen to bear interesting resemblances to the
spectra of the cube (Fig. 6a) and the octahedron (Fig. 6b), respectively. The Dyck graph is a bipartite trivalent graph like the cube and thus has the non-degenerate \( \pm 3 \) and degenerate \( \pm 1 \) values of the cube as well as the unexpected set of \( \pm \sqrt{5} \) eigenvalues of degeneracy 6. The Dyck graph dual, like the octahedron, has only three distinct eigenvalues, namely a non-degenerate \( +d \) eigenvalue, a doubly degenerate \( -\frac{1}{2}d \) eigenvalue, and a multiply degenerate 0 eigenvalue, where \( d \) is the degree of the equivalent vertices of the graph, namely 4 for the octahedron and 8 for the Dyck graph dual.

References


