INTRODUCTION TO TOP CRYSTALS

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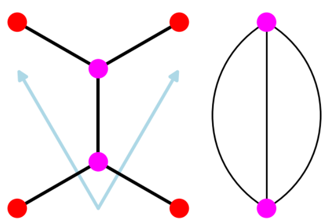
1. Brief idea of topological crystals

There are multiple fundamental domain for the same periodic graphs. However these fundamental domain correspond to different *quotient graphs*. A topolgical crystal (or periodic graph, as the graphene is) are *covering graphs* of quotient graphs. Any finite graph that is connected with no bridges, has a covering graph (no bridges means removing a single edge will not disconnect the graph).

For example here is another drawing of the fundamental domain of graphene (a fundamental domain has internal edges and external edges).



A finite graph can be equipped with a group (in particular which is a subgroup of something called the "first homology group" or fundamental group of the graph under some equivalence relation). This quotient graph subgroup combination corresponds uniquely pairs with a periodic graph (or topological crystal).

In the example of the two vertex fundamental domain of the graphene, its quotient graph equipped with its first homology group corresponds to it. If a fundamental domain corresponds to a quotient graph with its homology group, the periodic graph that fundamental domain produces is called a *Maximal abelian covering*.

There are unique conjectures pertaining to discrete periodic operators over such fundamental domains.

2. Some Graph theory

[1]

2.1. Introduction to graphs. A *graph* G (also called an undirected graph), is an ordered pair consisting of a set of *vertices* $V(G)$, and *edges* $E(G)$. We can write $G = (V(G), E(G))$ to represent G. Each edge e can be viewed as a pair of two vertices (u, v).

If we apply a geometric interpretation, then vertices u and v can be viewed as points in space, and edge $e = (u, v)$ is a segment with end points u and v.

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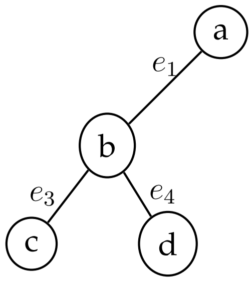
[1]Using Combinatorial Mathematics by Douglas B. West, whose class I sat in on for one day, liberally since it is very concrete and we are not setting out to be structural graph theorists (at least not me).

In a graph $G = (V(G), E(G))$, a vertex has an invariant called *degree*, denote $d(v) =$ the degree of v. The degree is the number of edges e of $E(G)$ that contain v.

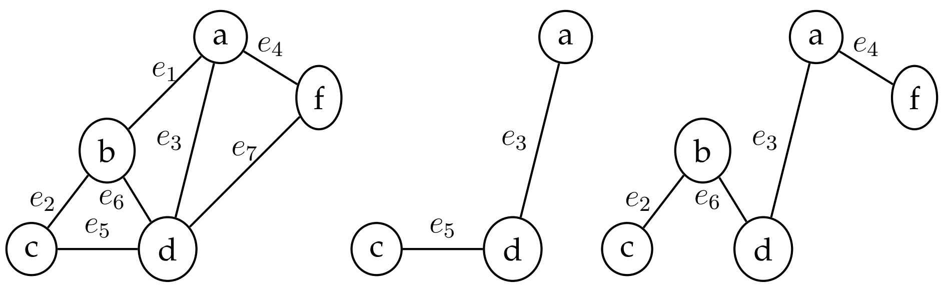


In this example b has degree 3 and all other vertices have degree 1.

A graph such that all vertices have the same degree is called *regular*.

A graph H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. A subgraph is called *spanning* if $V(H) = V(G)$.

Here is a graph, a subgraph, and a spanning subgraph



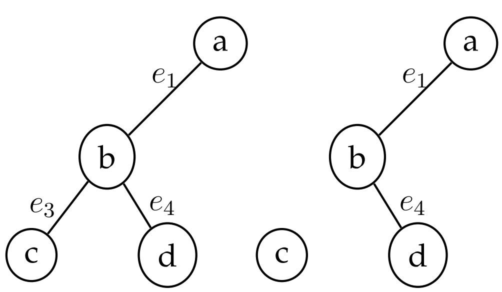
A **path** with n vertices is a graph who's vertices can be ordered $v_1 v_2 \ldots v_n$ such that (v_i, v_{i+1}) are edges of G. The nonspanning subgraph given above is the path abc. We can also write a path in terms of edges. In the example above the path from a to c can be written $e_3 e_5$.

A **cycle** is a path that starts and ends at the same vertex, for example looking at the first graph above $e_2 e_5 e_6$ is a cycle starting and ending at b.

A graph with no cycles is also known as a *Tree*.

A path $w_1 w_2 \ldots w_n$ for $w_i \in V(G)$ is called a u-v path if $u = w_1$ and $v = w_n$. A graph G is **connected** if a u-v path exists for all $u, v \in V(G)$.

A connected tree, and a disconnected subgraph:



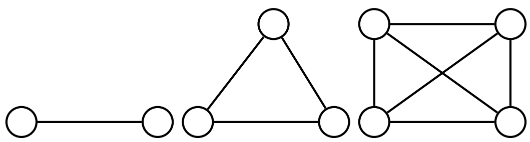
In a more abstract sense, we can view vertices as objects and edges as describing a relation between those objects. For example $(u, v) \implies u \sim v$ where $\sim$ is a symmetric relation. This relation $\sim$, can be denoted *adjacency*, in this way $\sim$ is not necessarily transitive nor reflexive.

If $u \sim v$ we say u and v are *neighbors*.

A graph is called complete if $\sim$ is an equivalence relation of and the vertices of the graph form an equivalence class of one element (if it is an equivalence class of multiple elements then it is a sum or union of multiple disjoint complete graphs). Another way to phrase this is, a graph is complete if it has as many edges as possible.

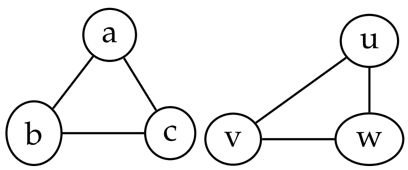
Complete graphs are unique up to the number of vertices, we denote K_n as the complete graph with n vertices.

For example here are K_2, K_3, and K_4.



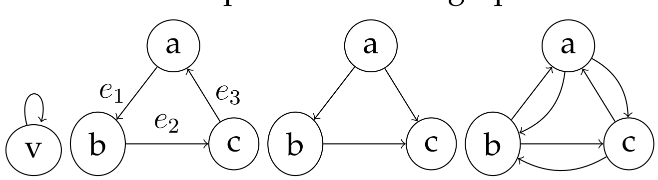
When I say unique, I mean up to relabeling of vertices and edges. Graphs are pairs $(V(G), E(G))$, a different geometric realization does not result in a different graph.

For example these two are the same graph K_3 (really this is to say these graphs are isomorphic, but for our purposes we will say they are the same).



2.2. **Directed Graphs.** A directed graph, or digraph, G is a pair of vertices $V(G)$ and edges $E(G)$ where edges are ordered pairs. In the previous section we talked about graphs, or undirected graphs an edge (u, v) was equivalent to an edge (v, u). In a directed graph these are distinct. Given a directed edge $e = (u, v)$ this denotes an edge from u to v. u is called the *tail* of e, and v is called the *head* of e. An edge $e = (u, u)$ is called a loop.

Are some examples of directed graphs.



Notice the last graph is such that if (u, v) is an edge, then it also has (v, u) as an edge, in this way this graph can be seen as a directed representation of it's undirected counter part.

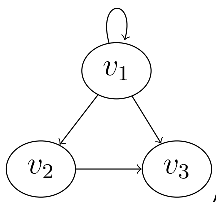
In the case of directed graphs, paths are still defined similarly, but are now subdigraphs. A path $v_1 v_2 \dots v_n$ exists if directed edges (v_i, v_{i+1}) exist. We see that the 2nd graph given above has a cycle $e_1 e_2 e_3$ where as the third graph does not.

Directed graphs have two notions of connectedness. Strong and weak. A digraph is *weakly connected* if replacing all directed edges with undirected edges results in a connected graph. A digraph is *strongly connected* if there is a directed path u to v for every ordered pair $u, v \in V(G) \times V(G)$.

u-v paths are defined in the same way. For example in the labeled graph above e_1e_2 is an a-c path, further this graph is strongly connected. The third graph shown above is weakly connected, but not strongly connected as there is no ac path.

A Digraph G can be represented by an adjacency matrix $Adj(G)$. We apply some ordering to our vertices $v_1, \ldots, v_n$. Then $Adj(G)$ is an $n \times n$ matrix of $0's$ and $1's$ such that $Adj(G)_{i,j} = 1$ if and only if (v_i, v_j) is an edge of $E(G)$.

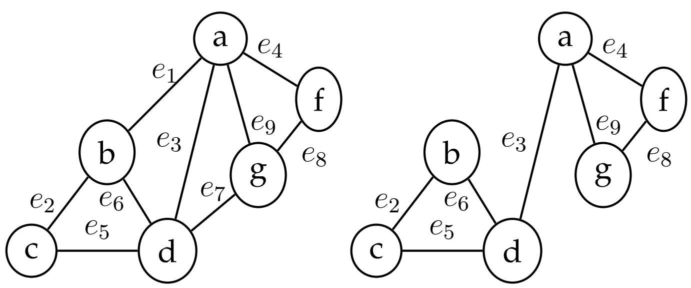
For example we have:

G = 

, and $Adj(G) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$

2.3. **Cut-edges.** An edge is a *cut-edge* or **bridge** if removing it disconnects the graph.

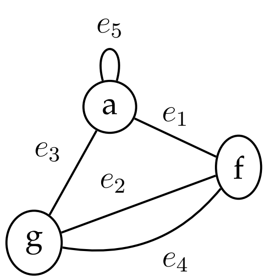
The first graph has no cut edges. The second graph does.



There is a lot more to be said about general graphs, but unless I think of more that should be more than enough for now. Let's move into our particular graphs.

2.4. **Our Graphs.** [2]

The quotient graphs we will be looking at are graphs where we allow for multiple edges between two vertices and loops (edges from a vertex to itself). Further all our graphs will be connected with no bridges.

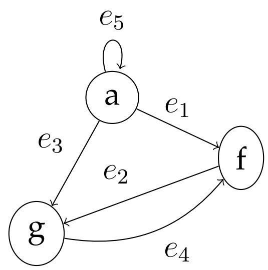


Our edges are a unique however in that we assign them an orientation of sorts. The choice of orientation does not have any affect on the objects we will obtain from our quotient graphs however which is why we do not just give a directed graph. Further this

[2]More on these with a more thorough treatment can be found in Sunada's Topological Crystallography.

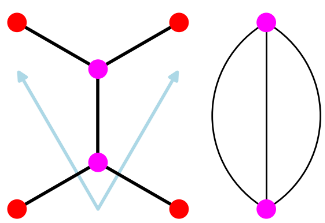
notion is distinct from a generic directed graph as we can traverse over an edge in either direction we just keep track of which direction.

Let us do an example by assigning an orientation to the example graph.



We let $\bar{e_i}$ represent traversing the edge in the direction opposite its orientation. For example we have paths from f-a paths $\bar{e_1}$; $e_2\bar{e_3}$; $e_2e_4\bar{e_1}$; $\bar{e_1}e_5$; $\bar{e_1}e_5e_5$; $\bar{e_1}\bar{e_5}$ and infinitely many more.

3. Topological crystals through Graphene 2 vertex fundamental domain example



So we talked a little about what these objects are called. Without going into too much detail (I will provide this later if there is interest). Let us see how the graphene is identified by this quotient graph.

In constructing a periodic graph from a quotient graph we first can start with something called a universal covering graph. To build this we identify vertices as paths (under an equivalence relation that is to be seen).

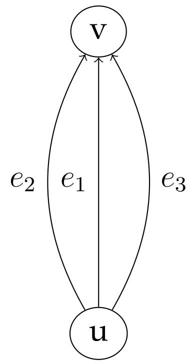
In the example below we have two vertices so we will just view e_i as an edge from u to v and its inverse $\bar{e_i}$ will take the same edge from v to u.

In this way we have paths u to v given by:

$[e_i]$, $[e_i\bar{e_j}e_k]$, $\ldots$ and so on.

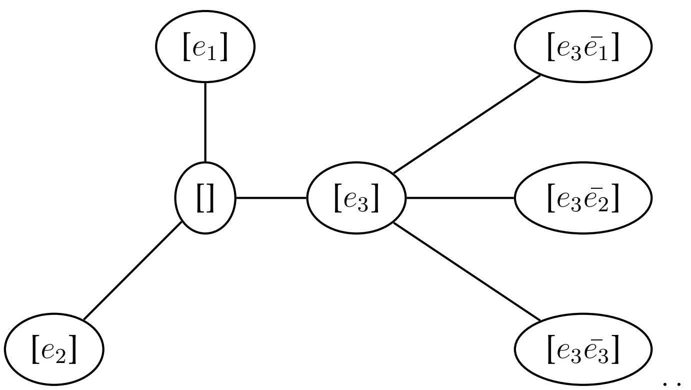
We also have paths u to u given by:

$[]$, $[e_i\bar{e_j}]$, $\ldots$ and so on.



A universal cover of a graph is an infinite graph where each path is assigned a vertex, and two vertices $[\gamma]$ and $[\beta]$ have an edge between them if there is an edge e such that $[\gamma e] = [\beta]$ where γ and β are paths written as a sequence of edges.

Here is the start of a universal cover of the example above (I will not include all as it is infinite so I cannot). Hopefully this is enough to get the general idea.



A maximal abelian covering can be obtained from a universal cover by imposing an equivalence relation on these paths.

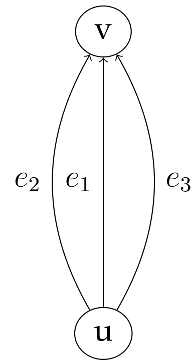
We say two paths $[\gamma]$ and $[\beta]$ are homologous, written as $[[\gamma]] = [[\beta]]$ if one can be obtained by another by the following:

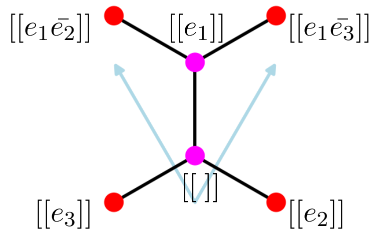
(1) Delete back tracking: that is if $[\gamma] = [\gamma_1 e_i \bar{e}_i \gamma_2]$ then $[[\gamma]] = [[\gamma_1\gamma_2]]$.
(2) Abelian loops that is if $[\gamma] = [\gamma_1\gamma_2\gamma_3\gamma_4]$ and γ_2 and γ_3 are loops (paths starting and ending at the same vertex) of the same vertex then $[[\gamma]] = [[\gamma_1\gamma_3\gamma_2\gamma_4]]$.

Under this relationship, the cycles based at u form a group called the *fundamental group* with composition on paths as the operation, that is $[[\gamma]] \circ [[\beta]] = [[\gamma\beta]]$.

Fixing the universal covering under this relationship gives us a maximal abelian covering.

Let us look at how our 2 vertex fundamental domain of graphene relates to this.





Notice that $[e_3\bar{e_3}]$ is no longer present (compare to universal cover) as $[[e_3\bar{e_3}]] = [[]]$

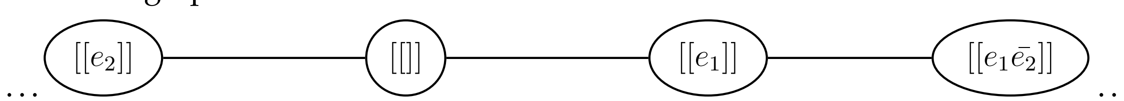
We notice that our action x takes $[[\,]]$ to $[[e_1\bar{e_2}]]$ and y takes $[[\,]]$ to $[[e_1\bar{e_3}]]$. These are both loops based at u. This is no coincidence, as these two loops also generate all loops based at u **Can you prove this?** These in fact are a generating set of the fundamental group of the quotient graph (or seed graph).

You might be wondering why we chose to place our vertices in such a manner, this is a good question. This is merely one of many "geometric realizations" of the maximal abelian cover of this quotient graph.

We can then get other graphs by imposing more equivalences (i.e taking quotient groups). For example we could set $e_1\bar{e_2} \simeq e_1\bar{e_3}$ and we would just get a graph that we could represent as a line with vertices, but this would still be identified with a 2 vertex fundamental domain of that linear periodic graph.

Since $e_1\bar{e_2} = e_1\bar{e_3}$ we have that $e_2 = e_3$

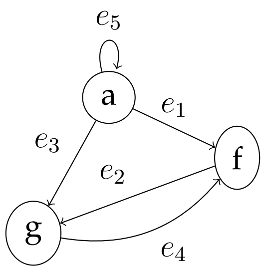
Thus this graph is as follows:



$[[]]$ and $[[e_1]]$ are taken as the fundamental domain, $e_1\bar{e_2}$ can be viewed as the action equipped to this graph.

In general we pair a quotient graph with a quotient group of its fundamental group and this will correspond to a particular fundamental domain of some topological crystal (also known as a periodic graph). We can always construct the fundamental group of a quotient graph as follows. We fix a vertex as the origin, lets say u, then the group of cycles that start and end at u give us the fundamental group. We write elements of the homology group as $[[\gamma]]$ where γ is a cycle starting and ending at u.

Let's do an example:



One way to know how many loops there are is, if the graph is planar (that is no edges are crossing), to count the number of distinct holes. In this case we have one from e_2e_4, one from e_5, and one from $e_1e_2e_3$. Thus we know the fundamental group will be generated by 3 elements. All we need is to choose generators that allow us to have cycles that only have each of these as holes in them and we have a generating set for the fundamental group.

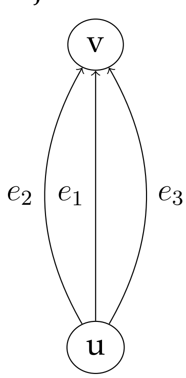
Let us fix a as the origin vertex. Then we can let $[[e_5]]$ be one generator, $[[e_1e_2e_4\bar{e_1}]]$ as another generator, and $[[e_1e_2\bar{e_3}]]$ as our final generator.

Exercise: Can you show these generators can produce the cycle $[[e_1\bar{e_4}\bar{e_3}]]$?

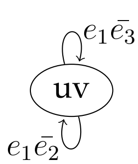
Hint: Generators also give you their inverse elements.

Example: $[[w\bar{x}]]^{-1} = [[(\bar{x})^{-1}(w)^{-1}]] = [[x\bar{w}]]$.

As Frank mentioned another way to know how many elements will be needed to generate the fundamental group is to contract edges until you have only a single vertex and then just count the loops:



Contracting e_1 this becomes



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