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Entangled Structures

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Contents

1 Abstract

This paper is a literature review in which methods used by various mathematicians and scientists to classify, understand, enumerate and represent different kinds of entangled structures are explored, explained and evaluated in the context of their wider applicability and usefulness in scientific fields that are highly concerned with entangled structures.

2 Introduction

Entangled Structures are ubiquitous in chemical and biological contexts where they can have major effects on the stability and chemical and biological function of certain structures. Some examples of this are enzymes such as topoisomerase that generate random entangled conformations of DNA plasmids as shown in Figure 1,

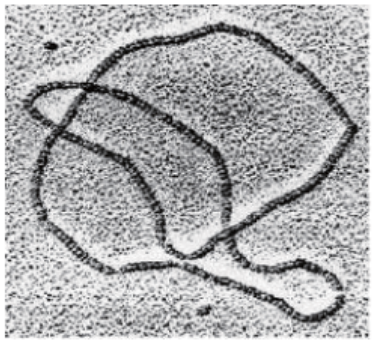

Figure 1: An Electron Micrograph of a trefoil knot formed from DNA. (Sumners - 2011)

or in periodic structures like Crystals and Metal-Organic Frameworks. Here we can see entanglement in the form of intrapenetration where a connected framework appears to entangle itself, or interpenetration where two or more connected frameworks thread through each other, as in Figure 2.

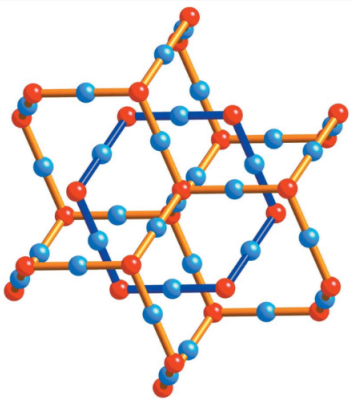

Figure 2: A segment of cuprite (Cu_2O) showing two interpenetrating structures. (Bonneau & O'Keeffe - 2015)

The prevalence of these entangled structures in scientific contexts creates a desire for a systematic way to classify, enumerate and understand these structures, in order to find connections between entanglement and the

physical, chemical and biological properties of these materials. This is something the language of mathematics is uniquely suited to address, but in order to have such a systematic approach we must be able to answer three main questions.

1. What is a suitable definition of entanglement?

   This is a very hard question to answer directly and so most of the approaches we will look at depend on identifying a class of structures as untangled and deciding that a given structure is entangled by showing that it is not the same as a member of this class. This methodology comes from the case of knots and links where we define the untangled class as all structures that are the same as a planar embedding of n disjoint circles, though in general, this approach is much more complicated. However, in order to use this definition, we have to ask,

2. How can we tell when two of these entangled structures are the same?

   In mathematics, the way we understand two objects to be the same is by defining an equivalence relation, $\sim$, which can be any method for identifying elements of a set with each other that obeys three rules; reflexivity (It must identify an object with itself $x \sim x$), symmetry (if $x \sim y$, then $y \sim x$) and transitivity (If $x \sim y$ and $y \sim z$ then it must be the case that $x \sim z$). Such an equivalence relation is then used to define subsets so that every element within the subset is identified with each other, and we call these subsets equivalence classes. We will discuss many examples of equivalence relations in this paper, but as there are a wealth of different equivalence relations it is important to understand which are the most useful for identifying the different kinds of entangled structures we are interested in. This connects to our final question when considering the many methods used to classify entanglement.

3. What are the best ways to classify/enumerate/represent these structures?

   Which will come down to the type of entangled structures we are considering, all the possible ways to classify each type of entangled structure and the relative advantages and uses of each type of classification.

This paper aims to explore and explain a variety of mathematical approaches to this problem of finding systematic ways to classify entanglement and will use the questions outlined above to guide our approach. We will then evaluate these classification methods based on how widely they can be applied to different kinds of entangled structures and how useful they are in generating deeper understanding of the entangled structures they apply to.

2.1 Statement of Authorship

As a literature review, none of the research presented in this paper is my own but has been collated by myself from a variety of sources given in the references section of this paper. I benefited greatly from discussions with my supervisor, Vanessa Robins, who helped guide my investigation and explain the significance and limitations of many of these approaches.

3 Spatial Graph Theory

In order to understand entanglement, we must first find a mathematical perspective that is generally applicable to our real-world examples of entanglement and this approach is often termed spatial graph theory (Flapan et al. - 2016).

3.1 What is Spatial Graph Theory?

Spatial graph theory is the study of embeddings of abstract graphs in a manifold. An abstract graph is a set $G = \{V, E\}$ where V is a set of vertices, $V = \{v_1, v_2, ...\}$ and E is a set of edges defined by pairs of vertices in V that each edge connects $E = \{[v_i, v_j], [v_k, v_l], ...\}$ (Rahman - 2017). These mathematical graphs represent an object by describing the connections between components of a set and are rarely thought of as physical objects. To give an abstract graph physical properties we consider embeddings in a manifold, $p : G \to X^3$. Here X^3 denotes an arbitrary 3-manifold like $\mathbb{R}^3, \mathbb{S}^3$ or $\mathbb{T}^3$ and p maps each graph vertex v to a distinct point $p(v) \in X^3$ and each edge $[u, v] \in E$ to the image of the interval $[0, 1]$ under some continuous function $f : [0, 1] \to X^3$ that satisfies $f(0) = p(u)$ and $f(1) = p(v)$. For a proper graph embedding we further require that the only intersections between embedded edges occur when the edges share a common endpoint. In this review we will generally only consider the space of proper graph embeddings following Power, Baburin & Proserpio (2020). We also note that we can place further restrictions on this notion of graph embedding by requiring that all edges be straight lines in X^3 which can be useful when considering the context of most crystallographic materials that are modelled by straight line connections between atoms.

3.2 Why Spatial Graph Theory?

We choose spatial graph theory as the lens through which we can understand entanglement because of its immediate connections to the scientific fields in which we typically find entanglement. As chemistry and biology are typically determined by connections between small structures via some bonding network, we can immediately see the appropriateness of the use of a graph to capture this bonding network in a variety of different contexts, whether in a crystal framework with atoms as vertices and covalent bonds as edges, in macromolecules like DNA where vertices are molecular groups and edges are Hydrogen bonds (Castle, Evans & Hyde - 2011) or even in the meta-structure of Metal-Organic Frameworks viewing metal ions or clusters as vertices and organic ligands or linkers as edges (Delgado-Friedrichs - 2004). Further, this approach is generally the most useful to study entanglement, as it sits between strict geometric equivalences, like congruence, which are inflexible to minor deformations in structure that occur constantly in biology and chemistry, and equivalence relations like topological homeomorphisms that do not care about the physical properties of the structure at all and only focus on the abstract connections between parts of the structure (Hyde & Delgado-Friedrichs - 2010).

4 Finite Graph Embeddings

Having now established our spatial graph theory perspective, we will first look at how we can understand the types of entanglement that occur in embeddings of finite graphs, which are any mathematical graphs with a finite set of vertices and edges. We will begin by first discussing how to determine when arbitrary finite graphs are the same, and use this definition, along with a variety of other methods to understand when a finite graph embedding is entangled and develop ways to classify arbitrary graph embeddings. We will conclude by looking at some special examples of entanglement known as knots, links and ravels, that can be better classified using more specialised methods.

4.1 Defining Entanglement through ambient isotopy.

The main equivalence relation used in spatial graph theory, which predominantly relies on ideas from topology, is that of ambient isotopy, and it is how we understand when two embeddings of an arbitrary finite graph are the same in terms of their entanglement.

4.1.1 What is Ambient Isotopy?

An informal definition of ambient isotopy is a deformation of an object that avoids edge and vertex collisions. It is also easy to think about making our object out of string and observing the ways we can deform the physical string embedding where we cannot pass the string through itself or totally collapse the string down to a point, but we do allow for the stretching and shrinking of segments of the string (Adams - 2004). A more formal definition relies on a notion of homotopy and homeomorphisms of topological objects. A homeomorphism is any continuous function between topological spaces $f : X \to Y$ with a continuous inverse $f^{-1} : Y \to X$ and a homotopy between topological objects is a family of continuous maps $f_t : X \to Y$ that define a single function $\Gamma : X[0, 1] \to Y$ given by the equality $\Gamma(x, t) = f_t(x)$ where Γ is continuous in both variables (Hatcher - 2001). We can then formally define an ambient isotopy as a homotopy of embedding functions $p_t : G \to X^3$, such that every embedding in the homotopy, $p_t(G)$, when viewed as a topological subset of the manifold, is a homeomorphism of the initial embedding, $p_0(G)$ (Johnson - n.d.). We can alternatively define this as a homotopy of the complement of the embedding in the manifold, which can sometimes be simpler to work with (Johnson - n.d.). Hence, if we take the space of all possible embeddings of a given finite graph and quotient out by the equivalence relation of ambient isotopy, we are left with a set of equivalence classes of structures with different kinds of entanglements, and we say representatives of these classes are isotopes of the graph embedding (Castle, Evans & Hyde - 2011). Due to the difficulty of defining entanglement directly, we opt instead to define a graph embedding as entangled whenever it is not in the same equivalence class as a known untangled embedding. However there are problems with this definition in that it doesn't give us any understanding as to when a structure is untangled and relies on the assumption that we will always be able to define an untangled embedding of an arbitrary finite graph.

4.1.2 Problems in Defining the Untangled Isotope

While many graphs would seem to have an obviously or intuitively untangled embedding, we need a rigorous definition of being untangled if we are going to use this to define when any structure is entangled. Unfortunately, there are graphs that do not admit any embeddings which are free of knots and links, suggesting that in these cases there are no intuitively untangled graph embeddings. Some examples of this are the complete graph on 6 vertices K_6 which has no embedding in $\mathbb{R}^3$ that is free of non-trivial links and the complete graph on seven vertices, K_7 which has no embedding in $\mathbb{R}^3$ that is free of non-trivial knots (Conway & Gordon - 1983).

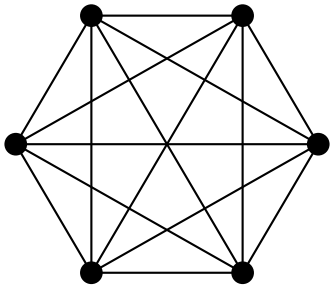

Figure 3: The complete graph on 6 vertices, K_6

This creates a complication in our goal of finding a way to define the untangled isotope of an arbitrary finite graph, as we are left with the choice to either say that some graphs have no untangled isotope, or we have to define an intuitively tangled graph embedding as the untangled isotope. This latter perspective may seem strange but it is useful when thinking of the untangled isotope as a minimal energy "ground state" embedding that can allow us to identify when a seemingly entangled object is actually just occupying the least tangled conformation available (Castle, Evans & Hyde, 2011). Such a ground state isotope for the complete graph on six vertices is shown in Figure 4.

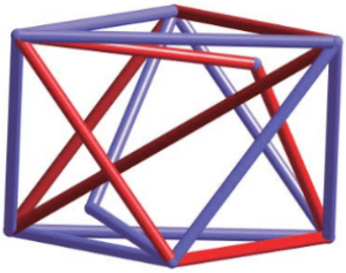

Figure 4: An "untangled" embedding of K_6 with a Hopf Link denoted in red. (Castle, Evans & Hyde - 2011)

Regardless of the perspective we take in order to approach this problem, it will be useful to find some way to rank graph embeddings that will work for all finite graphs. This will be useful in order to define an "untangled" or at least a "minimally entangled" isotope that we can easily refer to and will also generate a simple classification method that we can use to understand the patterns of entanglement in all finite graph embeddings.

4.2 Classifying arbitrary finite graph embeddings

We will begin our search for a ranking system that is applicable to all finite graphs by first considering the minimal genus embeddings of these graphs and then using a variety of energy functions to create a finer ranking of isotopes. Unfortunately, there is a degree of arbitrariness in our choice of ranking function, and generally the ranking functions chosen will not agree with each other. This means that while these ranking systems are universally applicable amongst finite graphs, they aren't inherently meaningful, and the choice of ranking function should be dependent on the context of the materials we wish to use this mathematical framework to study.

4.2.1 Minimal Genus Embeddings

The first step of our ranking function will be ranking isotopes by the minimal genus surface that the isotope can reticulate. We begin by noting that for this we are only considering compact, orientable 2D surfaces which by the Classification Theorem for Surfaces we know are unique up to a given genus g (Ghrist - 2014). The genus of a 2D surface can be colloquially thought of as the number of topological holes in the surface and we will mainly focus on the 2-sphere which has genus 0 and the torus which has genus 1. We embed a graph on a surface by considering the standard embedding of a compact, orientable, genus g 2D surface in Euclidean 3-Space, and create an embedding of a graph that places the vertices and edges of the embedded graph entirely on the embedding of the surface so that there are no edge crossings. This embedding is a reticulation if the complement of the embedding in the surface is a disjoint set of 2-cells that are homeomorphic to disks (Castle, Evans & Hyde - 2011). We therefore define the minimal genus embedding of a graph as the lowest genus surface which can be reticulated by the graph (Hyde & Delgado-Friedrichs - 2010). We can further extend this definition so that the minimal genus embedding of an isotope of the graph is the lowest genus surface that the isotope can reticulate. If the minimal genus embedding of a graph is 0, then by Whitney's Theorem, the embedding of this graph which defines the reticulation of the sphere is unique up to ambient isotopy (Castle, Evans & Hyde - 2011). Therefore a reticulation of the sphere by a particular graph can be used to define the untangled isotope of the graph as there is no lower genus than 0 and the isotope that reticulates the sphere is unique if it exists. Unfortunately there are many graphs which cannot reticulate the sphere and so may have many non-isotopic reticulations of the same minimal genus surface. We therefore require different techniques in order to distinguish between these different isotopes that reticulate each surface. This is important both in order to define the single untangled isotope of a graph if we would like one to exist, and to further classify all isotopes of a graph in some increasing order of complexity. It is at this point that we turn to energy functions in order to rank the different isotopes after we have sorted them by the minimal genus surface that each isotope can reticulate.

4.2.2 A 3D Energy Function

All information in this section comes from Evans, Robins & Hyde (2015). There are many different kinds of energy functionals of graphs that allow us to classify their embeddings by some measure of their complexity but we will quickly describe one such method which is a generalisation of the rope-length embedding of knots to arbitrary finite graphs. The Rope-length functional of a knot is the minimal length of rope required to realise the knot, divided by the diameter of the rope used. We also call this the tight embedding of a knot or graph. We can use a numerical algorithm SONO (Shrink-On-No-Overlaps) to realise this embedding for knots, but not graphs as there needs to be specific considerations made for many edges coinciding at a vertex which will have collisions for any thickness of rope no matter how well spaced they are around the vertex. These considerations have been made in the numerical algorithm PB-SONO (Periodic-Branched-Shrink-On-No-Overlaps) which builds on the ideas in the SONO algorithm, gives similar results for knots as SONO and can also be used to give finite graph embeddings an energy defined by $E_{3D} = \frac{L}{D}$ Where L is the total length of all edges in the embedding and D is the largest diameter circle that the embedded edges can be expanded out to without overlapping. Some examples of this energy function applied to untangled, linked and knotted cubic graphs is shown in Figure 5.

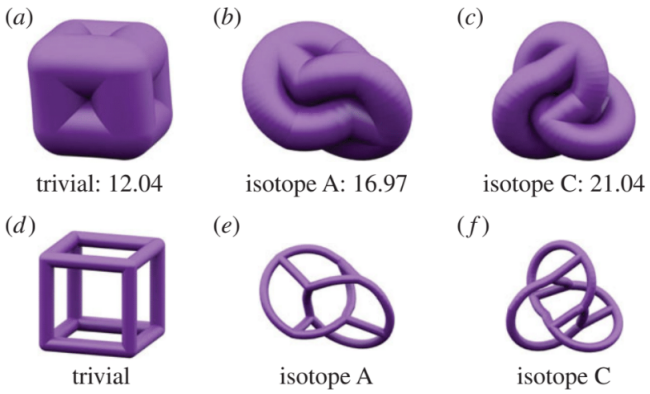

Figure 5: Tight Embeddings (with expanded and normal edges) of Untangled, Linked and Knotted Isotopes of the Cubic Graph and their respective energies, E_{3D}. (Evans, Robins & Hyde - 2015)

4.2.3 A 2D Energy Function

Another kind of Energy function we can consider for a graph isotope uses the minimal genus embedding of the isotope to generate a 2-dimensional energy function. We begin by taking the reticulation of our minimal genus surface by our graph, and lifting this pattern to the universal cover of the surface which is $\mathbb{R}^2$ for the torus and the hyperbolic plane for all higher genus surfaces. (We are ignoring the sphere in this energy function because if a graph isotope can reticulate the sphere, then we know it is the unique isotope with this property and so doesn't need further categorisation). We find that these surface reticulations will lift to periodic patterns in the universal cover, and we can find a barycentric placement for this periodic pattern in the universal covers (Castle, Evans & Hyde - 2011). These barycentric placements are defined so that each vertex is in the average position of all of its adjacent vertices or more explicitly the embedded vertex $p(v)$ is given by

$$p(v) = \frac{1}{|N(v)|} \sum_{w \in N(v)} p(w)$$

Where $N(v)$ is the set of all vertices adjacent to v (Delgado-Friedrichs - 2004). We also note that Barycentric placements exist for every connected 2-periodic graph and are unique up to affine transformation (Delgado-Friedrichs - 2004), making them useful for defining this energy functional. We then create our energy functional by looking at a unit cell of this periodic pattern in the universal cover that corresponds to the isotope we started with and then summing the square of the length of all edges in the unit cell in the universal cover, so $E_{2D} = \sum_i l_i^2$ where l_i is one of the edge lengths (Castle, Evans & Hyde - 2011).

Therefore, we have shown that we can classify entangled structures represented by any finite graphs by taking the space of embeddings of a given graph, quotienting out by the equivalence relation of ambient isotopy to find a set of isotopes of the graph, initially ranking these isotopes in order of the lowest genus surface that each graph isotope can reticulate and then further delineating the isotopes that can reticulate the same genus surface and no smaller genus surfaces by some energy function. These energy functions are unfortunately quite arbitrary and will generally lead to conflicting rankings of isotopes. However, they are still useful as they can be applied to any finite graph embedding, and a particular researcher can simply use the most sensible ranking function for their perspective.

In addition to this universally applicable method for ranking the entanglement of arbitrary finite graphs there are certain kinds of entanglement for which we can have more systematic kinds of enumeration and classification that lead to deeper insights into the nature of their entanglement but cannot be broadly applied. We will look at some of these methods for knots, links and ravels.

4.3 Knots and Links

We can consider the study of knots and links as a form of spatial graph theory, where we are looking at embedding $n \geq 1$ copies of the single vertex, single edge graph, but this perspective can be limiting as it does not allow for the generalisation of knots to higher dimensions (Sumners - 2011), and ignores other properties that can be used to distinguish knots and links. Consequently, knot theorists tend to use a variety of different techniques to classify knots and links, the most common of which is their crossing number, which is the smallest number of crossings from any projection of any embedding in the isotopy class of the knot (Sumners - 2011). However, like the minimal genus embedding of a graph this is insufficient to characterise knots as there are generally many knots with the same crossing number. We also have some simple classifications for different kinds of links notably Hopf links, which are two interlocked loops whose minimal crossing number is 2, and Brunnian links which occur when 3 or more loops are interlocked in such a way that the removal of any one loop would cause the whole structure to become untangled (Adams - 2004). More detailed descriptions of knots and links come from algebraic topology, where polynomial invariants of knots, such as the Alexander polynomial can be derived from a set of algebraic rules applied to oriented embeddings of knots (Conway - 1967). Further, there are different equivalence relations we can use to group certain knots together such as cobordance, which

deems two knots to be equivalent if there exists an embedding of an annulus $\mathbb{S}^1 \times [0, 1]$ in a 4-dimensional space, bordered by two parallel 3-dimensional spaces, such that the loops $\mathbb{S}^1 \times \{0\}$ and $\mathbb{S}^1 \times \{1\}$ become embeddings of the knots in the two 3-dimensional boundary spaces (Conway - 1967).

While these approaches are very valuable in the field of algebraic topology and are also incredibly interesting, they aren't terribly useful for categorising knots in applications as they lack a certain intuitiveness. However, many of these algebraic ideas have been used to create a very succinct arithmetic of tangles that can be used to systematically enumerate knots. The basic method from Conway (1967) involves finding a set of basic polyhedra, which are planar graphs where every vertex is of degree 4 and no region of the plane is bordered by two vertices and two edges, then substituting various tangles into these vertices and simplifying our expression according to a set of known equivalences. The advantage of this notation is in its computability, its applicability to all kinds of knots and links and the visual intuition that it creates without even knowing much about the notation due to the connection between the numerical notation and the kinds of crossings in the knot , see Figure 6.

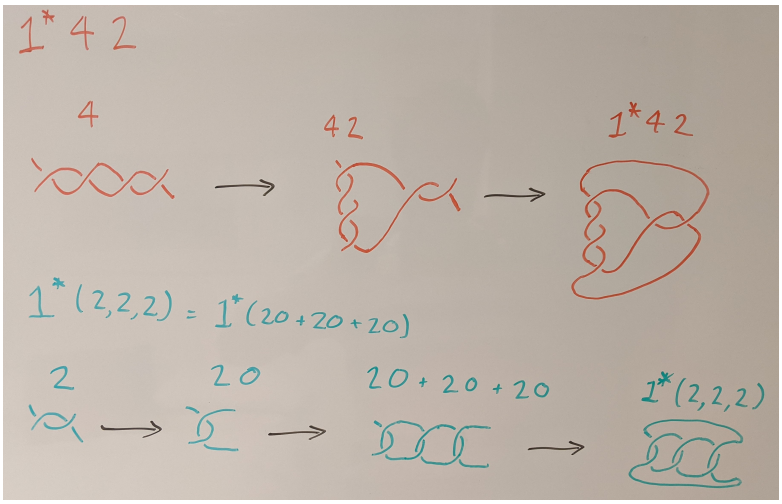

Figure 6: A Hand Drawn knot and link using Conway's notation.

So, in summary we have a large variety of tools to describe, characterise and enumerate knots and links that have different strengths such as creating deeper understanding of the inherent properties of knots in the case of polynomial invariants, generating understanding of higher dimensional embeddings in the case of cobordance and in general communicability as with Conway's notation.

4.4 Ravels

All information in this section is sourced from Castle, Evans & Hyde (2008). While we have discussed knots and links quite a lot as they are often viewed as the simplest form of entanglement and are an easily identified, intuitive indicator of entanglement, there is a known type of entanglement of finite graphs that is free of knots and links which has been termed ravels. Ravels are a vertex localised form of entanglement that can be substituted into embedded graphs by replacing a local neighbourhood of a vertex of appropriate degree with a particular ravel in order to generate an entangled structure that contains no knots or links. We require the

degree of the vertex at the centre of a ravel to be greater than two as this helps ensure that the closure of the ravel remains unknotted as long as every strand coming from the vertex is required for the entanglement, and as the entanglement is only around the vertex, these structures are free of links as any two cycles formed by closing the edges in the ravel must share a vertex and hence cannot be disjoint cycles which are required for links. We can classify ravels as universal if the closure of the edges of the ravels at a common second vertex creates a tangled structure, and selective if a closure of the dangling strands of the ravel that is not all at the same vertex creates an entangled structure. We can further describe ravels as fragile if the removal of any edge from the ravel causes the whole structure to disentangle, composite if it can be formed by smaller ravels via edge contraction or similar operations or shelled if the ravel can be formed by substituting the local neighbourhood of the vertex at the centre of a ravel with a ravel. These classification methods are useful for understanding how ravels form entanglement and while there are certain topological invariants that have been found for certain classes of ravels like those in θ-graphs, there is still work to be done in order to thoroughly classify ravels.

Figure 7: A ravelled tetrahedral graph (Hyde & Delgado-Friedrichs - 2010)

5 Periodic Graph Embeddings

We now turn our attention to periodic graph embeddings and the different methods that have been employed to characterise, enumerate and represent periodic entanglement. The notable difference between these representations, compared to finite graph embeddings, is that we usually make the simplifying assumption that all edges between embedded vertices are straight lines as this more closely resembles the physical realities of crystal-like structures. There are notable exceptions to this including the use of PB-SONO to characterise periodic graph embeddings and rod packings in Evans, Robins & Hyde (2015), and the embedding of ravels in periodic structures in Castle, Evans & Hyde (2008), but from now on, we will be adding in the assumption that an embedded periodic graph has its edges $[u, v]$ defined as the unique straight line between the embedded vertices, $[p(u), p(v)]$ where p is the embedding function on the set of vertices (Power, Baburin & Proserpio - 2020).

5.1 Representations of Periodic Graphs

5.1.1 What are Periodic Graphs?

A d-periodic graph is a simple undirected graph on which the group $\mathbb{Z}^d$ acts by graph automorphisms such that the group action is free, which immediately implies that the vertex set is countable and the degree of each vertex

is finite (Delgado-Friedrichs - 2004). When considering periodic graph embeddings we will typically require the embedding to also be periodic, which allows us to view the action of $\mathbb{Z}^d$ on the abstract graph as instead being a set of translations of the embedding by integer copies of d basis vectors that define the directions of periodicity, which we call the periodic structure basis $\underline{a} = \{a_1, a_2, ..., a_d\}$ (Power, Baburin & Proserpio - 2020). We note that these basis vectors will define a unit cell given by the set $\{t_1a_1 + t_2a_2 + ...t_da_d |\ t_i \in [0, 1)\}$ that we can imagine as a tiling of our ambient space such that each tile can be mapped onto any other tile by translating by a vector of the form $k_1a_1 + k_2a_2 + ...k_da_d$, where $k_i \in \mathbb{Z}$. We will call these periodic embeddings with straight line edges, linear periodic nets (Power, Baburin & Proserpio - 2020).

5.1.2 Quotient Graphs and Labellings

All the information in this section is sourced from Power, Baburin & Proserpio (2020). We can use the group action of $\mathbb{Z}^d$ to define a finite set of orbits on the vertex and edge sets with which we can construct a quotient graph whose vertex set is the set of orbits of vertices under the action of $\mathbb{Z}^d$ on the graph and the set of edges becomes the set of orbits of edges where the endpoints of the edges are redefined to be the orbits that the original vertices belong to. This means if there were two edges that connected one vertex to two different vertices that were in the same vertex orbit, our quotient graph would have two distinct edges between the same pair of vertices. Similarly, if an edge connected two vertices that were representatives of the same vertex orbit this would generate a loop edge in the quotient graph, which connects a vertex to itself. We will often use the action of $\mathbb{Z}^d$ to add labels to the graph, generating a labelled quotient graph. The labelled quotient graph is easier to understand from the perspective of the embedded periodic structure where we have a representative of each vertex orbit in every tile of our manifold which are defined above as the translations of $\{t_1a_1 + t_2a_2 + ...t_da_d |\ t_i \in [0, 1)\}$ by integer copies of the periodicity basis vectors, and the label of an edge in the quotient graph is a vector $(k_1, k_2, ..., k_d) \in \mathbb{Z}^d$ which denotes the coefficients of the translation required between the two cells that the edge connects. So if an edge connected two vertices in the same unit cell that edge in the labelled quotient graph would be denoted $(0, 0, ..., 0)$. If the edge connected one vertex to a vertex in a tile that was one translation in the direction a_1 away, then the label on the edge would be $(1, 0, ..., 0)$ and similarly for translations in any other basis vector directions. While these quotient graphs and labelled quotient graphs are not indicators of entanglement, they are useful as a way of categorising our linear periodic nets.

5.1.3 Linear Graph Knots in $\mathbb{T}^3$

All the information in this section is sourced from Power, Baburin & Proserpio (2020). We can also consider the result of rescaling our embedded periodic net so that the periodic structure basis is the standard basis $\{e_1, ..., e_d\}$. which is achieved by the action of a change of basis matrix on the whole embedding space which we will assume is $\mathbb{R}^d$. This means our unit cell is now $[0, 1)^d$ and if we quotient $\mathbb{R}^d$ by the action of $\mathbb{Z}^d$ on this unit cell, and equip it with the quotient topology we are left with what is known as the flat d-torus. We will now focus solely on the case of embeddings in $\mathbb{R}^3$ becoming embeddings in the flat 3-torus, $[0, 1)^3$. Using this

perspective we can simplify an infinitely periodic net to what is known as a linear graph knot in the flat 3-torus which we can think of as a cube with periodic boundary conditions. This is equivalent to considering the space of embeddings of labelled quotient graphs in the flat 3-torus, where the labels determine how many times the straight line edges pass through the periodic boundaries and which boundaries they pass through.

We will quickly note that there are always multiple choices of periodicity basis we could use for this construction when given a particular linear periodic net, and while we often choose a periodicity basis $\underline{b} = \{b_1, b_2, ..., b_d\}$ such that the lattice defined by the points by the points $k_1b_1 + k_2b_2 + ...k_db_d$, where $k_i \in \mathbb{Z}$ is maximal amongst all choices of periodicity basis. We call such a basis and the linear graph knot generated by these bases, primitive. However, there are certain contexts in which we want some flexibility in our choice of basis, and so we do not require the choosing of a primitive periodicity basis in the construction of quotient graphs, labelled quotient graphs and linear graph knots in the flat 3-torus.

5.2 Defining Entanglement of Periodic Graphs

Now that we have some general terminology of periodic graph embeddings, we can now concern ourselves with how mathematicians describe the entanglement of these periodic structures and the many difficulties involved in these approaches.

5.2.1 Generally Applicable Methods.

We can transfer some of the methods from the finite graph case to this problem. The 2D Energy function described earlier can be adapted to periodic graphs which can be thought of as reticulations of surfaces of unbounded genus (Castle, Evans & Hyde - 2011). The universal cover of these surfaces is also the hyperbolic plane and if our graph embedding is crystallographic, meaning the automorphism group of the graph is isomorphic to one of the crystallographic space groups (Klee - 2004), we can use a similar technique to generate a ranking function, though there is some degeneracy in the use of this technique to help define untangled embeddings meaning we can end up with multiple "untangled" isotopes. (Castle, Evans & Hyde - 2011). We can similarly use PB-SONO to help characterise these periodic embeddings (Evans, Robins & Hyde - 2015). While these approaches are generally applicable we would also like to have methods that are more illuminating to the specific features of periodic structures and related areas of mathematics.

5.2.2 Heegaard Splittings

One such method that highlights interesting properties of periodic graphs is that of Heegaard Splittings. We can consider the linear graph knot representation of the linear periodic nets in the flat 3-torus as the spine of a handlebody obtained as a regular neighbourhood of the embedded graph. If the boundary of this handlebody creates a Heegaard Splitting of the flat 3-torus, then the boundary surface is defined as unknotted (Bai et al. - 2017) and we can consequently use this fact to define the spine of the handlebody as untangled. This approach to entanglement agrees with our general intuition, as nets that are universally accepted as being untangled like

pcu and **dia** fit this definition. However, this approach has more interesting applications as these Heegaard Surfaces in the flat 3-torus create triply periodic minimal surfaces like the P surface and diamond surface, creating a link between the defining pattern and symmetry of triply periodic minimal surfaces and untangled net embeddings. This can lead to further insights as it is known that all Heegaard Splittings generated by handlebodies of genus $g \geq 3$ are unique up to isomorphism, and as the P surface, the diamond surface and gyroid are all defined by genus 3 handlebodies splitting the 3-torus, there is a form of isomorphism between them (Boileau Otal - 1990). This approach can also be used in the case of finite graphs, where we consider the embeddings of the finite graphs in the 3-sphere that generate Heegaard splittings as untangled (Johnson - n.d.).

While this method is interesting for the connections it provides, there are more easily computable ways to find and classify entanglement in periodic structures.

5.2.3 Periodic Isotopy

As we often restrict our focus to embeddings of periodic graphs that form linear 3-periodic nets, the equivalence relation of ambient isotopy can give too much flexibility to the space of embeddings we are considering, and so for ease of computation and enumeration we can restrict to the equivalence relation of periodic isotopy. We say that two linear periodic nets $\mathcal{N}_0, \mathcal{N}_1$ are periodically isotopic if there is a family of nets $\mathcal{N}_t$ for $0 < t < 1$ for which there is a continuous path of bases of $\mathbb{R}^3$, $t \to \underline{a}^t$, $0 \leq t \leq 1$ where $\underline{a}^t$ is a right-handed periodic basis for $\mathcal{N}_t$ and there are bijective functions $f_t : \mathcal{N}_0 \to \mathcal{N}_t$ for $0 \leq t \leq 1$ which map vertices to vertices such that f_0 is the identity map on $\mathcal{N}_0$ and for each vertex $p \in \mathcal{N}_0$ the map $t \to f_t(p)$ is continuous (Power, Baburin & Proserpio - 2020). We note that as each edge is the unique straight line between the embedded vertices, the continuous transformation of the edge positions is immediately determined by the continuous change in vertex positions (Power, Baburin & Proserpio - 2020). This notion of equivalence is perhaps the most thorough way to classify embeddings of given periodic graphs but is still computationally difficult due to the sheer number of possible embeddings, we note that there are 19 periodic isotopy classes of the highly restricted category of connected linear 3-periodic nets in $\mathbb{R}^3$ with a single-vertex quotient graph whose labels are of the form (x_1, x_2, x_3) where $x_i \in \{-1, 0, 1\}$ (Power, Baburin & Proserpio - 2020)

5.2.4 Cycles, Rings, Strong Rings and Essential Rings

A more easily computed way to find and describe entangled structures involves analysing the cycles of a periodic graph for the presence of knots and links. While the absence of knots and links doesn't necessarily imply a structure is untangled, as we saw with ravels that can be embedded in periodic graphs (Castle, Evans & Hyde - 2008), their presence in periodic graphs doesn't imply the structure is entangled either. This is because knots and links can be found in all periodic structures including the primitive cubic network **pcu** (Hyde & Delgado-Friedrichs - 2010). To remove this confusion, we must look for knots and links in particular kinds of cycles in the periodic graph and so we require some definitions. A cycle is any closed path that begins and ends at the same vertex and we will assume these cycles are elementary, which means that no edge or vertex appears in the path

more than once (excluding the starting vertex) (Delgado-Friedrichs & O'Keeffe - 2005). Cycles are added by adding the edges in the two cycles equipped with $\mathbb{Z}/2\mathbb{Z}$ coefficients, so if an edge occurs an even number of times in the sum it is excluded, and if it occurs an odd number of times in the sum it is included (Delgado-Friedrichs & O'Keeffe - 2005). We then define a ring as a cycle that is not the sum of two smaller cycles and a strong ring as any cycle that is not the sum of any number of smaller cycles (Delgado-Friedrichs & O'Keeffe - 2005). We then note that if a net admits a natural tiling, which is a tiling such that the edges of the tiles are the net and the tiles themselves have the same space group symmetry as the net, then the cycles that define the faces of the tiling can be called essential rings of the structure and it is conjectured that these essential rings form a ring basis in the sense that any other cycle can be formed by adding together some number of these rings (Bonneau & O'Keeffe - 2015). This terminology allows us to classify different levels of self-entanglement that can occur in nets by observing what kinds of cycles form links in the net. The ranking proposed by Bonneau & O'Keeffe (2015) goes from trivial self entanglement where only cycles that aren't rings are catenated, to weak rings being catenated, strong rings being catenated and then ends with the essentially self-catenated networks that have catenated essential rings. This method while somewhat limited to nets that admit natural tilings does allow for a more systematic kind of ranking of self-catenating structures.

5.2.5 Classifying Types of Catenation

However, self-catenation is not the only kind of entanglement we can consider as we can also have two or more disconnected structures interpenetrating in certain patterns of catenation. A very simple way to begin to classify general kinds of catenation is by listing the overall periodicity of the entangled nets followed by the periodicity of the connected components, so interpenetrating cubic nets would be denoted $\{3 : 3\}$ whereas rod packings would be denoted $\{3 : 1\}$ and so on (Power, Baburin & Proserpio - 2020). This method is not terribly useful for any detailed classification of structures but is a good step in restricting a study to a certain type of interpenetrating structure and can be further refined by looking at parallel, inclined, homogeneous, heterogeneous, shift homogenous and transitive subcategories of interpenetrating nets (Power, Baburin & Proserpio - 2020).

5.3 Utilising Symmetry

The inherent symmetry of an abstract graph is described by its automorphism group, but graph embeddings are described by their space group (See Appendix). We can define a maximally symmetric embedding of a graph to be one whose space group is isomorphic to the automorphism group of the graph and we know that these maximally symmetric embeddings correspond to minimal energy placements of vertices (Power, Baburin & Proserpio - 2020). When these minimum energy placements are free of edge collisions we call these embeddings stable, and these embeddings are unique up to spatial congruence and rescaling making them good representatives for untangled graph embeddings for a particular periodic graph. However there are more uses for symmetry than just providing good representations of particular periodic isotopes, we can also use them to create novel catenated structures and classify the symmetry of interpenetration.

5.3.1 Using Sub/Super-Group Relations to find Interpenetrating structures

A methodology descrbied by Baburin (2016) shows how we can use an embedding of a net $\mathcal{N}$ with a space group H that has a supergroup G such that the index of H in G is n to generate n interpenetrating copies of the same net. We note there are some limitations to the kinds of supergroups allowed such as, there may be no mirror plane symmetries in G that are not already in H and any axes of rotation in G that are not in H must not pass through any of the edges or vertices of $\mathcal{N}$, thus reducing the number of super groups that need to be considered. We can also apply this technique to subgroups of the space group of our maximally symmetric embedding to generate entanglements of nets including traditionally cubic embeddings like **pcu** or **dia** having interpenetrating nets with hexagonal space groups. While this method is quite limited in its applications for characterising entangled embeddings, it is a highly useful and informative description of the types of possible embeddings in this class of entangled structures using the language of group theory.

5.3.2 Hopf-Ring Nets and the Symmetry of Interpenetration

Another interesting use of symmetry to describe entanglement is through the Hopf-Ring Net described by Alexandrov, Blatov & Proserpio (2012). Here we take a given net embedding and define a new net by placing vertices at the barycentres of certain strong rings in our initial net that form a ring basis of the structure and then adding edges whenever two of those strong rings form Hopf-links. We can then study the maximally symmetric embedding of this new net to understand the symmetry of the interpenetration pattern of our initial net embedding. This method is especially useful in the realm of cycle analysis as it can be applied to networks that do not necessarily admit natural tilings, and while there may be many different nets with the same Hopf-Ring Net it is still a useful tool to help delineate between different kinds of entangled embeddings.

6 Discussion and Conclusion

Overall, this paper has shown that there is a very broad range of ideas and approaches that have been employed by mathematicians over the years in order to better understand, categorise and explore the world of entangled structures, with varying levels of success and general applicability in the approaches undertaken.

7 Appendix: Space Groups

A space group is a group of isometries of some Euclidean space $\mathbb{R}^n$ that leave a given crystal pattern invariant, where a crystal pattern is a set of points in $\mathbb{R}^n$ such that the translations that leave the points invariant form a vector lattice in $\mathbb{R}^n$ (Souvignier - 2008). These isometries are all affine transformations that can be represented by augmented matrices like

$$\left[\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]$$

Where the upper left submatrix is a linear transformation in $\mathbb{R}^n$, the upper right submatrix is a vector translation and the lower submatrices are just placeholders required so that the multiplication of these augmented matrices is a proper representation of the group composition (Souvignier - 2008).

Space Groups are generally constructed by a set of translations, a point group which is a set of linear transformations like rotations, reflections and inversions, and combinations of these two operations that generate glide symmetries (affine transformations consisting of mirror reflections and translations) and screw symmetries (affine transformations consisting of rotations and translations) (O'Keeffe & Hyde - 1996). We will often represent these symmetry operations using the points, lines and planes that act as the axes of symmetry for these operations (O'Keeffe & Hyde - 1996).

We categorise these space groups by restrictions on their unit cell which apply to different crystal systems which are, triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, cubic and then denote these space groups using a letter that describes the type of lattice present in this unit cell as well as a symbol denoting the point group symmetries that are present in the unit cell (O'Keeffe & Hyde - 1996).

As noted in Baburin (2016) the boundaries of this classification are fuzzy as there is a trigonal space group which is a subgroup of both a hexagonal supergroup and a cubic supergroup, which have no subgroup/supergroup relationship between them. This is what allowed for the creation of interpenetrating cubic nets with a hexagonal space group defining the maximal symmetry embedding.

8 Appendix: Heegaard Splittings

All this information comes from Johnson (n.d.). To understand Heegaard Splittings we must first define handlebodies. Let $B_1, ..., B_n$ be a collection of closed balls and let $D_1, ..., D_m, D'_1, ..., D'_m$ be a collection of pairwise disjoint disks in $\bigcup \partial B_i$ For each $i \leq m$ let $\phi_i : D_i \to D'_i$ be a homeomorphism. Let H be the result of gluing these balls along ϕ_1, then ϕ_2 and so on. If H is connected then H is a handlebody. (The process of gluing involves quotienting the whole set by the equivalence relation that treats two points $x \in D_i, y \in D'_i$ as equivalent if $y = \phi_i(x)$ or equivalently $x = \phi_i^{-1}(y)$ which we know exists as ϕ_i is a homeomorphism).

Next we will define a barycentric subdivision. First we consider a simplicial complex $K = (V, F)$, where V is a set of vertices and F is a collection of sets of vertices that define the faces of the simplicial complex with the property that if $\{v_1, v_2, ..., v_n\} \in F$ then any subset of this set is also in F. A barycentric subdivision of a simplicial complex $K = (V, F)$ is another simplicial complex $K' = (V', F')$ such that $V' = F$ and F' consists of all subsets $\sigma \subset V'$ such that for some ordering we can write $\sigma = \{a_1, a_2, ..., a_n\}$ where a_j is a face of a_i whenever $j > i$. We call repeated applications of this procedure the second, third, fourth etc. barycentric subdivision of a simplicial complex.

If we have a piecewise linear graph embedded in a 3-manifold, we can find a triangulation of the manifold that contains the graph as a subcomplex of the triangulation. This means there exists a simplicial complex, K, which is a triangulation of the manifold M, such that the homeomorphism $\phi : K \to M$ maps some subcomplex $A \subset K$ to the piecewise-linear graph embedded in the manifold. We then consider the second barycentric subdivision of this complex, K'' and define $A'' \subset K''$ to be the subcomplex such that the canonical map $\psi : K'' \to K$ maps $A'' \to A$. We now define the set $N = \{\sigma \in F'' | \sigma \cap A'' \neq \emptyset\}$ and call the set $\phi(\psi(N)) \subset M$ the closed regular neighbourhood of our piecewise linear graph embedding. If this regular neighbourhood is a handlebody, we call our graph embedding the spine of the handlebody it creates.

A Heegaard Splitting of a 3-manifold, M is an ordered triple (Σ, H_1, H_2) where Σ is a closed surface embedded in the manifold, H_1 and H_2 are handlebodies embedded in M such that $\partial H_1 = \Sigma = \partial H_2 = H_1 \cap H_2$ and $H_1 \cup H_2 = M$. We call Σ a Heegaard surface.

For this paper we are concerned with linear graph knots embedded in $\mathbb{T}^3$ that are the spines of handlebodies whose boundary is a Heegard Surface in $\mathbb{T}^3$. If this is the case we say that the net defined by this linear graph knot in the flat 3-torus is untangled.

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