Entanglements of polyhedral graphs and three-periodic nets

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We are interested in enumerating and classifying tangled embeddings of finite and infinite graphs. Infinite graphs arise from three-periodic nets in crystal chemistry, see for example [1] and `rscr.anu.edu.au`. A long-term goal is to enumerate and classify sensibly nets via edges of tilings of three-periodic minimal surfaces (the EPINET project; see [2], `epinet.anu.edu.au`). The discovery of "tangled" embeddings of well-known nets (e.g. **dia**, the diamond net [1], discussed in [3]) inspired us to study the issue of entangled embeddings of (finite) graphs and nets. Following the EPINET philosophy – where we explore 3D euclidean embeddings via reticulations – drawings of edges without crossings – of 2D oriented manifolds – we have chosen to analyse entanglement similarly.

Denote a graph embedding of a graph G in 3-space, up to ambient isotopy, $\mathcal{G}_g^i$ where g denotes the minimum genus of the associated oriented 2-manifold that can be reticulated such that the resulting edge pattern in 3-space is $\mathcal{G}_g^i$ and the index $i \in \{1, 2, \ldots, n\}$, corresponding to the n distinct embeddings of that genus (where n may be infinite).

Suppose $G \subset P$, where P is a polyhedral graph (3-connected, simple and planar). Here any $\mathcal{P}_0^1$ that reticulates the 2-sphere (genus zero) is untangled (and Whitney's Theorem ensures that $n = 1$). We define the simplest entanglements of P to be those examples $\mathcal{P}_1^i$ that reticulate the 2-torus (genus one). Among those $\mathcal{P}_1^i$, we rank them from least to most entangled by forming a canonical embedding on the flat torus, via barycentric placement of the associated 2-periodic euclidean planar graph. As the degree of entanglement (in this definition) rises, the ratio of total edge length to area of the flat torus increases. The simplest examples of tangled polyhedral graphs $\mathcal{P}_1^i$ (where $i \lesssim 20$), sorted by a model energy have been enumerated for the cases where G corresponds to the tetrahedron, octahedron and cube graphs [4, 5].

Assuming that all toroidal polyhedra contain knots or links, we have proven that *all* toroidal polyhedral embeddings are chiral [6].

We extend this idea to more complex graphs, G. In other words, for a graph embedding $\mathcal{G}_g^i$, first find the minimal-genus g; increasingly tangled embeddings of G are $\mathcal{G}_{g+1}^j$, $\mathcal{G}_{g+2}^k$, $\ldots$. We sort embeddings $\mathcal{G}_h^i$ with equivalent minimal-genus h by ordering via the ratio of edge length to manifold area of the graph in a canonical reticulation in the manifold, again generated by forming the barycentric periodic graph in the universal cover (now the hyperbolic plane), giving a ranked sequence $\{\mathcal{G}_h^1, \mathcal{G}_h^2, \mathcal{G}_h^3, \ldots\}$. Examples for $g > 1$ have not yet been explicitly calculated, though we think there are no fundmental obstacles.

Consider lastly the case where G embeds as a three-periodic infinite net (whose minimal-genus, $g = \infty$). In this case, we suggest, barycentric embedding of G in 3-space [9] as the untangled state. This prescription will occasionally fail, but it affords the usual embeddings of simpler nets at least. Whether this definition corresponds to the untangled net generated as the limit of a sequence of graphs whose minimal genus approach ∞, we do not know.

These basic ideas will be published shortly elsewhere [10].

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