# SCULPTING ENTANGLEMENT

### STEPHEN T. HYDE AND ROBERT OWEN

## 1. INTRODUCTION

Ten years ago, Peter Harrowell, a chemical physicist at Sydney University, sent SH \* an image of a sculpture he had seen at the Art Gallery of NSW, shown in Fig. ??(a). This is one of a series of sculptures made then and since by RO.

I was kind of intrigued

Peter wrote,

this is an eight vertex 3-fold net with the topology of a cube yet it clearly is entangled - a sort of self interpenetration (sounds a bit unsavoury).

SH too was intrigued and wondered how that form related to the more usual *cube graph*, with its six squares loops, joined three by three. Within the language of graph theory, it was indeed an embedding of the cube graph, with 12 vertices, all of degree three, and its topology was indeed that of the cube (Figure ??(b)). For example its "coordination sequence" - an integer sequence that describes the number of vertices reached from a root vertex, is  $\{1, 3, 3, 1\}$ . This is pretty clear from a drawing of the cube graph of Figure ??(c).

Peter Harrowell's key observation – at least to SH at the time – was that the structure was "entangled", with a threading of edges through the quadrilateral cycles, giving rise to knots in the embedding. Here was an extraordinarily beautiful, yet conceptually simple example of a phenomenon that SH had been thinking about in a far different context for some time, stimulated by a fascinating observation from another colleague, Davide Proserpio, a structural chemist in Milan. He noted that the structural skeleton of a complex metal-organic framework material, appeared to be topologically identical to diamond: its (infinite) coordination sequence and cycles matched those of the diamond net, well known to all solid state scientists (as, for example, the covalent bonding framework in actual diamond, with  $sp^3$  carbon atoms at the vertices). Yet this "diamond" net was also entangled, and could

<sup>\*</sup>Here we abbreviate the authors as SH (Stephen Hyde) and RO (Robert Owen)



FIGURE 1. (a) RO's sculpture Vessel #2 from the series "Cubes and Hypercubes" (2003). Photo, Art Gallery of NSW, Robert Owen, Different Lights Cast Different Shadows, 2004. (b) Standard "untangled" embedding of the cube graph in 3-space. (c) Representation of the cube graph in the extended complex plane (the three outermost vertices are glued to give a single vertex.

(b)

(c)

only be realised from the usual diamond pattern by breaking bonds, and rethreading them through cycles, changing the crossing order of edges in projection. This was a beautiful example of a self-entangled network pattern; far more complex than more familiar knots (which can be analysed as entangled loops). But classification of this tangled diamond pattern seemed hopeless: it was a union of an infinite set of branched knots, rather than a simple knot or link, and there was no privileged projection from 3-space to the two-dimensional plane that simplified the entanglement.

In contrast, RO's *Hypercube*, with just eight vertices and twelve edges, was far more manageable; an elegant and possibly tractable example of a more generic and utterly unexplored phenomenon: entanglement of a relatively simple finite graph, that of the cube.

#### 2. TANGLED CUBES

RO's constructions in *Hypercube* and related sculptures, such as the *Florentia* models (Figure ??), though each geometrically different, are nevertheless topologically equivalent to the cube graph, all sharing the cube coordination sequence. They can be bundled into two genera: those that can be deformed into the usual Platonic form of the cube graph in three-space by a sequences of movements that change only edge lengths and vertex angles, and those whose homeomorphisms require edges to pass through each other to form the standard cube, thereby changing the mutual threading or edges. The former are "untangled" and the later "tangled" cubes. Untangled polyhedral graphs, like the cube, are readily defined in topological terms: they are (in the language of graph theory) "planar embeddings" and can be traced on the surface of a sphere  $(S^2)$  via an "ambient isotopy" that does not require phantom crossings of edges through each other. In contrast, tangled examples cannot be untangled without allowing edges to pass through each other.



FIGURE 2. Robert Owen's *Models for Florentia* (painted steel), 2006.

For some time, SH called these tangled cases "knotted cubes". The analogy is clear: mathematicians define knots as embeddings of loops  $(S^1)$  that cannot be morphed into the "unknot" (that can be drawn in the plane without crossings) without phantom crossings, and so knots cannot be unknotted without cutting and reconnecting the loop. Like all graphs, cube graphs can be thought of as branched loops (with branch points at their vertices). So understanding of tangled graphs, like RO's tangled cubes, seemed to demand extension of the tools of knot theory to branched knots. Perhaps then, a useful ranking of tangled nets, including Owen's cubes and Proserpio's metal-organic framework, could be constructed from concepts in knot theory. Given the complications of knot theory, that task alone was daunting enough, but worth exploring. A simple scalar measure of knot complexity is a "knot energy", introduced by Fukuhara ? and O'Hara ? as analogues of electrostatic arrays, and Moffat ? from the viewpoint of fluid dynamics. Since then, various formulations of knot energies have been explored ?, ?

An interesting route to that goal was the notion of "tight knots". This approach was appealing in its physical aspect, in contrast to the more abstract algebraic invariants of knot theory, such as the celebrated Conway and Jones polynomials?. Tight knots are embeddings of knots that minimise the knot arc length, assuming the knot is a flexible tube with uniform thickness, imposing excluded volume constraints. A useful, though not unique, ranking of knot energies is related to the ratio of arc length to thickness, the "ropelength". This idea has been explored from the late 1990s, in mathematical contexts. Its applications of physics are many and varied, from "glueballs" of high energy physics ?, to gel electrophoresis of knotted DNA ? and the breaking strength of good old-fashioned physical knots ?! A useful numerical algorithm that often – though not always – converges to a likely shortest ropelength is the SONO algorithm ?. A number of deep and more widely applicable questions surround the notion of knot energies, and a sensible definition of such an energy. For example, we can ask whether the most symmetric embedding of a knot in three-space is one of lowest energy? For many definitions of the energy, the answer is often no. Tight knots, in contrast, are often realised as very symmetric objects.

The SONO algorithm was extended by Myf Evans, while she was a PhD student with SH and Vanessa Robins, to the "PB-SONO" algorithm, in order to explore tight embeddings of graphs (or branched knots) ?. Here too the results were encouraging, since (in particular) relaxed embeddings of simple unknotted graphs, like the unknotted cubes, were equivalent to those of the familiar structures of symmetric Platonic cube edges (Figure ??a). Better still, knotted examples of simpler nets, like RO's cube graphs, converged readily to fixed configurations (Figure ??b).

Most encouraging of all, relaxed embeddings of infinite periodic nets were virtually indistinguishable from the canonical barycentric embeddings (with maximal volume and equal edge lengths) realisable by Olaf



FIGURE 3. (a), (c) Untangled and tangled A-type cube isotopes. (Note the edge crossings.) (b), (d) Tight configurations of the untangled and A-type tangled cubes, calculated by Myf Evans ?.

Delgado Friedrichs' and Mike O'Keeffe's equilibrium placement algorithm ?. If these relaxed untangled nets converge to geometries of the most symmetric barycentric embeddings, it is surely reasonable to impose the same energy on tangled nets, and rank their entanglements by their ropelength. It seemed, then, that a quantitative handle on the degree of complexity of Proserpio's "tangled diamond" net was in sight.

But further exploration of tangled graphs forced us to think more deeply about entanglements.

#### 3. TANGLED GRAPHS

Our assumption that entangled graphs were really just branched knots (or links) was rudely shattered by construction of an entangled *theta* graph, illustrated in Fig. ??(a). Evidently, this embedding is tangled, as the loops are threaded and cannot be separated. But all loops are themselves unknotted. Further, we cannot locate tangled links in

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the embedding composed of multiple loops whose vertices belong to one loop only. (Try it!) This example demonstrated that entanglements in graphs can be more complex than generalised branched knots. Here was a new entanglement motif that had no counterpart in knots (or links). We called this motif a *vertex ravel*, since it is localised to the (three) edges emanating from a single vertex; one could contain it within a ball centred on that vertex ?. (We later realised that this specific ravel was known to knot theorists, and had in fact been described earlier by Kinoshita ?.) The existence of ravels means that the phenomenon of tangling in graphs is a more complex issue than that of knots alone. Given the mathematical difficulties of knot theory itself, explication of entanglement of graphs is evidently a complex challenge.

This example allowed SH and his students to construct extended families of ravels or various types ?, which we proposed as potential entangled structures in materials, particularly framework materials, such as the tangled diamond structure described by Proserpio et al. Entanglement in these materials is unsurprising, since their structural networks contain long, polymeric edges, whose capacity to intertwine grows with their length. To our surprise, a first "ravelled" framework molecule was synthesised and recognised shortly afterwards by Australian chemists, in a metal-organic material ?.



FIGURE 4. (a) An entangled *theta* graph: a simple *vertex ravel*. (b) Embedding of the ravel on a genus-two *bitorus*. (c) Embedding of the ravel on a genus-three *tritorus*. The ravelled *theta* graph cannot be embedded on the (genus zero) sphere, or the (genus one) torus without edge crossings.

Why was the ravel so complex? In contrast to the untangled polyhedral graphs, that embed in the (genus-zero)sphere, and the simpler tangled polyhedral graphs, that embed in the (genus-one) torus, the ravel appeared to reticulate only in a more complex topological object, namely the genus-two *bitorus* and more complex manifolds (Fig. ??(b)). The addition of "handles" to the topologically simpler sphere and torus, to form the bitorus (or tritorus) allows the graph edges to mutually entwine sufficiently to form a ravelled embedding. This surface reticulation suggests a novel approach to classification of entangled graphs, namely their exploration as reticulations of underlying two-dimensional manifolds. And advances in tiling theory in recent years?,?,? can be adopted to systematically enumerate reticulations of two-dimensional surfaces of arbitrary topological complexity. Thus, for example, polyhedral graphs can be enumerated (to an arbitrary degree of complexity) via enumeration of tilings of the sphere. And we can likewise enumerate tangled polyhedral graphs by exploring tilings of the genus-one torus, the genus-two bitorus, etc. A first classification of the complexity of a specific entanglement follows from the (lowest) genus of the underlying two-dimensional manifold (assumed for now to be oriented for simplicity) that can be reticulated to form that tangled embedding.

This approach led to a first enumeration of the simplest tangled cubes by exploring embeddings of the cube graph on the torus ?. In particular, SH chose to enumerate simpler distinct isotopes – all cube graphs, but with distinct entanglements of edges that cannot be morphed into each other via ambient isotopies – with equal faces on the torus. The imposed condition – supposed wrongly to be a natural constraint for any cube isotope – was that no cycle be longer than the largest non-intersecting cycle in the cube itself, namely the Hamiltonian cycle with eight vertices. Since the cube graph has degree-three vertices, this constraint amounts to enumerating less wound tilings of the torus by the graphene  $(\{6,3\})$  net, containing just eight vertices. Five such examples were found, four of which can be readily drawn with straight edges. Recall that the conventional (untangled) cube has six square faces, forming a (topological) cube. These five simplest tangled cubes – from the "A-type" to the "E-type" cube – contain just four hexagonal faces, wrapped on a torus. One family of embeddings, whose curved edges are derived from the underlying torus geometry, is shown in the top row of Table ??. Equivalent entangled forms can be produced by many different geometric embeddings. Some examples with straight edges for the A- to D-type cubes are illustrated in row 2 of the Table.

The "tangled cube" constructions of RO can also be classified within this taxonomy. Thus, for example, Vessel #2 and some (though not all) of the *Florentia* constructions are A-type cubes. Examples of both A-type and untangled cubes are listed in Table ??.

As a result of the catalogue of straight-edges A- to D-type cubes, RO constructed a number of new cubes, entangled and untangled, moulded to give more aesthetically powerful embeddings. That process is one that – like the mathematical analysis of torus embeddings described above – morphs between three and two dimensions. RO's tangled constructions emerge by the following processes. First, a three-dimensional euclidean embedding of a graph, such as a conventional cube, is projected to the plane (two-dimensional euclidean space). Vertices are then moved around in the plane, then fixed, settling their  $\{x, y\}$  coordinates. Their z coordinate in (euclidean three-dimensional) space is then chosen by fixing a height on vertical sticks placed at the  $\{x, y\}$  sites. Evidently, this operation need to preserve the entanglement of the initial embedding.

More recently, a new series of cube constructions were built by RO, via the same project method. Some of those newer constructions however, were made from initial embeddings that were themselves tangled, namely the straight-edge embeddings illustrated in the second row of Table ??. Once again, the entanglements of the initial embeddings were not necessarily maintained during the process. The resulting *Thought Form* constructions depict a wider spread of tangled forms, from the untangled case, to A- to C-type cubes, listed in Table ??.

That topological approach to enumeration of toroidal polyhedral graphs led to a comprehensive enumeration of tangled tetrahedral, octahedral and cube graphs via embeddings in the torus by Toen Castle ?. This enumeration removed any constraints on largest cycles, revealing an infinite universe of possibilities. Once again, RO's work provided some inspiration. SH had noticed many examples of unidentified tangled polyhedra among the sculptures in RO's studio. At a glimpse, these appeared to be tangled dodecahedra. Now systematic enumeration of toroidal tangles of dodecahedra is a tricky computational task, given the size of the dodecahedral edge graph (with 20 degree-three vertices). Nevertheless, with some clever analysis, Toen reduced the computational task to manageable size, and eventually found two families of toroidal dodecahedra, albeit both containing both large and small faces on the torus, in contrast to the simplest toroidal cubes (whose faces – on the torus – are all hexagons).

An example of a complex "dodecahedron" constructed by RO is shown in Figure ??. This convoluted spatial form, devoid of evident spatial symmetries or regular geometry of any type, writhes and twists through space hypnotically. Its coordination sequence is identical to that of the dodecahedron, and fixed, regardless of which of the twenty vertices we choose as the "root vertex", namely,  $\{1, 3, 6, 6, 3, 1\}$ . This

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TABLE 1. (Top row) The four simplest entangled toroidal cube graphs that can be drawn with straight edges in 3-space. (Second row) Embeddings of the simplest tangled cubes with straight edges. (Lower rows) RO's constructions of cube graphs, from the *Vessel, Florentia* and *Thought Form* series. Some correspond to tangled cubes, others are untangled.

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is the coordination sequence of the dodecahedron (Figure ??(c). This construction is therefore a tangled dodecahedron. Its subtle geometry is more complex (and beguiling to the human eye) then either the conventional regular (untangled) Platonic dodecahedron, or any of the toroidal tangled dodecahedral isotopes found by Toen Castle. It is a tangled polyhedral isotope whose complexity is beyond our enumerative capabilities at present. It seems certain that it embeds on a torus of genus at least two, but the lowest genus torus that can be reticulated to form this particular isotope is unknown.





FIGURE 5. (a) Robert Owen's dodecahedron construction, Carbon Copy #2, from the series "Different Lights Cast Different Shadows" (2003). Photo, Art Gallery of NSW, 2004. (b) labelled by a coordination sequence from an arbitrary vertex, labelled "0". (c) Planar drawing of the dodecahedron edge graph, revealing its coordination sequence:  $\{1, 3, 6, 6, 3, 1\}$ .

One further construction by RO is worth exploring through this graph theoretic prism, since it illustrates another subtle aspect of entanglement in nets. *Florentia Bloom 2*, is shown in Figure ??. This construction embodies a graph with 18 degree-three vertices, so it is clearly not a dodecahedron, tangled or otherwise. Its coordination sequence depends on the choice of root vertex; one case is shown in Figure ??(b)). We cannot trace this graph within the plane without edge intersections; at least one pair of intersecting edges results (Figure ??(c)). Indeed, we can trace the degree-three bipartite graph,  $(K_{3,3})$  as a subgroup of this graph. One choice is shown in Figure ??(d). Kuratowski's Theorem guarantees that this graph is therefore topologically non-planar ?, so it is no surprise that it cannot be drawn on the page without intersecting edges. It is therefore also certainly not a tangled polyhedral graph, since these are (topologically) planar. But is it tangled?

This is a subtle question, that can be answered in a number of ways. In our view, it can only be answered by first defining an untangled "ground state" for this (non-polyhedral) graph. Since the graph drawing of Figure ??(c) has just one crossing of edges, it can be drawn on the surface of a (genus-one) torus without crossings. The torus "handle" – not present on the sphere – allows sufficient freedom for the crossed edges to be separated. Since the graph is non-planar, this is the lowest genus (oriented) manifold which can be reticulated to give this construction. It cannot be further disentangled to reduce edge crossings. In our view then, it is "untangled", despite its complex threaded structure. This feature is common to all non-planar graphs. Classification of their entanglement is therefore a delicate issue, and much work remains to arrive at useful signatures for these non-planar cases.

Nevertheless, our analysis (via mathematics) and construction (via sculptural art) of entangled polyhedral (and therefore planar) graphs offers a useful starting point for that study. This tale exemplifies an often overlooked synergy between the creative arts/sciences/ Both authors - scientist and artist – have been exploring related ideas independently and occasionally in tandem, with very different languages of form. Yet beneath these superficially disparate approaches lies a common goal: exploration of space.

### 4. LOOKING FURTHER

We have chosen to emphasise simpler entanglements, constructed from mathematics and visual experiments. The dialogue described here, between the analyses from topology, graph and tiling theory, and



(a)



FIGURE 6. (a) Robert Owen's Florentia Bloom 2. (Image courtesy of Robert Owen.) (b) Construction labelled by a coordination sequence. (c) Planar drawing of the graph topology of this construction, with a single edge crossing. Edges are coloured to mimic the coloured edges of (a) and vertices are labelled by their index in the coordination sequence (as in (b)). (d) A  $K_{3,3}$  sub-graph found within the graph of (c), with (non-trivial) degreethree vertices of  $K_{3,3}$  coloured cyan and red. (e) The bipartite  $K_{3,3}$  graph.

the constructions allowed by morphing polyhedral nets projected into two euclidean dimensions, then lifting back into three, is an open one. RO has a wealth of other constructions that are equally intriguing to explore from the perspective of polyhedral entanglement. Melburnians and Sydneysiders can explore this without too much effort.

Visitors to Hamer Hall in the Arts Centre need only look to the ceiling in the entry, to find *Silence* made of seven suspended crystalencrusted sculptures: all dodecahedra. Their various entanglements have yet to be explored. The high-rise Triptych apartment building looms just behind the Arts Centre. This building too is decorated with some of RO's tangled polyhedral constructions. (The coloured decorations on the external walls are also designed by RO.) Another series of seven variously-tangled dodecahedra, *Axiom* decorate the atrium of the Commonwealth Law Courts in 305 William Street.

Sydney is also home to a number of readily accessible RO sculptures. A suite of tangled polyhedra entitled New Constellation hang in the foyer of the MLC Building in Martin Place (along with a large RO painting). RO's most complex form is on public view, across the harbour, and just behind Luna Park, at Harry's Park, adjacent toot eh offices of the late Modernist architect, Harry Seidler. This large sculpture, Tracing Light - For Harry 3D/4D replicates RO's procedure of planar projection followed by lift back into three-dimensional space described above. But here the initial object is a four-dimensional polyhedron, a hypercube, or tesseract. Entanglement of this graph is a still more complex issue!

#### 5. Acknowledgements

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#### References

- R. V. Buniy and T. W. Kephart. A model of glueballs. *Physics Letters* B, 576(1):127–134, 2003.
- T. Castle. *Entangled graphs on surfaces in space*. PhD thesis, Australian National University, 2013.
- T. Castle, M. E. Evans, and S. T. Hyde. Ravels: knot-free but not free. novel entanglements of graphs in 3-space. *New Journal of Chemistry*, 32:1484–1492, 2008.

- P. R. Cromwell. Knots and links. Cambridge University Press, 2004.
- O. Delgado-Friedrichs. Recognition of flat orbifolds and the classification of tilings in r<sup>3</sup>. Discrete and Computational Geometry, 26:549– 571, 2001.
- O. Delgado-Friedrichs and M. O'Keeffe. Identification of and symmetry computation for crystal nets. Acta Cryst. A, 59:351–360, 2003.
- A. W. Dress, D. Huson, and E. Molnár. The classification of facetransitive periodic three-dimensional tilings. Acta Crystallographica Section A: Foundations of Crystallography, 49(6):806–817, 1993.
- M. Evans. *Three-dimensional entanglement: knots, knits and nets.* PhD thesis, Australian National University, 2011.
- S. Fukuhara. Energy of a knot. A fête of topology, pages 443–451, 1988.
- D. H. Huson. The generation and classification of tile-k-transitive tilings of the euclidean plane, the sphere and the hyperbolic plane. *Geometriae Dedicata*, 47(3):269–296, 1993.
- S. T. Hyde and G. Schröder-Turk. Tangled (up in) cubes. Acta Cryst. A, 63:186–197, 2007.
- V. Katritch, J. Bednar, D. Michoud, R. G. Scharein, J. Dubochet, and A. Stasiak. Geometry and physics of knots. *Nature*, 384:142–145, 1996.
- S. Kinoshita. On elementary ideals of polyhedra in the 3-sphere. Pac. J. Math., 42:89–98, 1972.
- C. Kuratowski. Sur le probleme des courbes gauches en topologie. Fundam math, 15(16):271–283, 1930.
- F. Li, J. K. Clegg, L. F. Lindoy, R. B. Macquart, and G. V. Meehan. Metallosupramolecular self-assembly of a universal 3-ravel. *Nature Comm.*, 2:205, 2011.
- H. K. Moffatt. The energy spectrum of knots and links. Nature, 347:367–369, 1990.
- J. O'Hara. *Energy of knots and conformal geometry*, volume 33. World Scientific, 2003.
- J. Ohara. Energy of a knot. *Topology*, 30(2):241–247, 1991.
- P. Pieranski. In search of ideal knots. In A. Stasiak, V. Katritch, and L. H. Kauffman, editors, *Ideal Knots*. World Scientific, Singapore, 1998.
- P. Pieranski, S. Kasas, G. Dietler, J. Dubochet, and A. Stasiak. Localization of breakage points in knotted strings. *New Journal of Physics*, 3(1):10, 2001.
- R. G. Scharein. Interactive topological drawing. PhD thesis, Citeseer, 1998.

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