

Mobility of ‘ N -loops’: bodies cyclically connected by intersecting revolute hinges

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Abstract

The mobilities of many objects from toys and molecular models to large scale deployable structures can be understood in terms of N -loops: sets of N bodies, cyclically connected by pairs of intersecting revolute hinges. A symmetry-extended version of the Grübler criterion for counting kinematic degrees of freedom is used to explain and rationalise the observed mobilities of N -loops with small N . Compared to simple counting, the symmetry based approach gives improved detection and visualisation of mechanisms and states of self-stress. It can also give a better account of the differing mobilities of conformers occupying different regions of the phase-space, such as the rigid chair and flexible boat forms of cyclohexane.

1 Introduction

Mobility counting and rigidity theory provide concepts that are used and re-used in contexts from conformational analysis of small molecules (Dunitz and Waser, 1972), mechanics of protein structures (Jacobs et al., 2001), modelling of pH-dependent expansion of nano-scale viral particles (Kovács et al., 2004), through robotics (Porta et al., 2009), to generation of designs for deployable engineering structures (Chen et al., 2005). Many systems at these

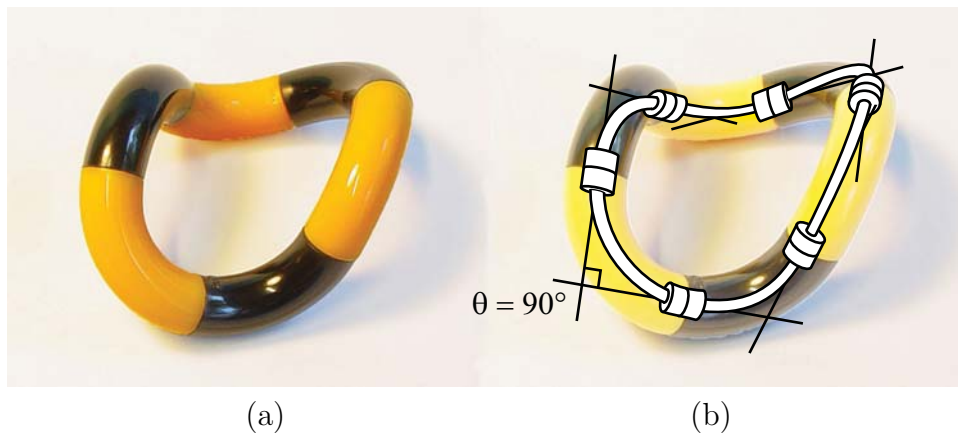


Figure 1: (a) Tangle model of the 6-loop in the twist-boat conformation; (b) line drawing showing bodies, hinges and intersecting hinge-lines. The angle of intersection is $\theta = 90^\circ$.

different length scales can be described as cycles of bodies linked by intersecting revolute hinges. The present paper is concerned with the mobility of such cycles, and in particular, with the kinematic insights that can be gained by exploiting symmetry.

We define an N -loop as consisting of N rigid bodies, linked in a cycle by joints, such that each joint is a revolute hinge allowing torsional freedom about a line, and such that the two hinge lines for each body intersect. All distances between neighbouring intersections, and all angles of intersection are allowed, and indeed much of our treatment will be applicable to this general situation. However, in applications, the configurations of interest are usually *regular* $N(\theta)$ -loops, in which all distances between neighbouring intersections are equal, and all intersection angles are equal to some angle θ (which is taken to be greater than or equal to $\pi/2$).

The ‘Tangle’ toy (<http://www.tanglecreations.com>) provides a simple means of building tangible realisations of N -loops with $\theta = 90^\circ$ that allow exploration of their mobility properties. Figure 1 shows one conformation of a 6-loop constructed from Tangle pieces, together with an analysis in terms of the bodies, hinges and hinge-lines of the N -loop description.

The interesting properties of Tangles have been used as the basis for educational workshops in mathematics (Freudenthal, 2003). Constructing and handling Tangle models (Figure 2) leads to a number of immediate observations:

$N = 4$ As $\theta = 90^\circ$, a 4-loop can be constructed in a planar conformation

(Figure 2(a)), but the physical model allows small out-of-plane deformations without apparent distortion of the components.

$N = 5$ It proves to be impossible to assemble a regular 5-loop with $\theta = 90^\circ$. It is easy to show by a geometrical argument (Freudenthal, 2003) that it is not possible to close a chain of five 90° ‘elbows’ and simultaneously align the hinges.

$N = 6$ There are two ways in which a 6-loop can be constructed from Tangle pieces. One leads to a rigid conformation (Figure 2(b.i)). The other leads to a family of non-rigid conformations lying on a one-parameter pathway. The two high-symmetry conformations are shown in Figures 2(b.ii,iii). To convert from the rigid to a non-rigid conformation of the Tangle model requires dismantling and re-assembly. The three illustrated models are $\theta = 90^\circ$ equivalents of the three well-known conformations of cyclohexane (see below).

$N = 7$ There are also two ways in which a 7-loop can be constructed from Tangle pieces, but now both lead to one-parameter families of non-rigid conformations, and passage from one family to the other is possible only by dismantling and re-assembly. Figures 2(c.i,ii) show high-symmetry points on the path connecting chair-like conformations, whilst Figures 2(c.iii,iv) show high symmetry points on the path connecting boat-like conformations. The four illustrated models again have their equivalents in molecular conformations (of cycloheptane) (Crippen, 1992; Graveron-Demilly, 1977).

$N = 8$ Figure 2(d) shows three conformations of a Tangle model of an 8-loop. All are interconvertible, in what is clearly a multi-parameter family. Porta et al. (2007) show that for cyclooctane (an 8-loop with θ equal to the tetrahedral angle, $\theta_T = \cos^{-1}(-1/3) \approx 109^\circ 28'$), all conformations form a single interconnected family.

$N > 8$ Some examples of loops with larger N are discussed in Freudenthal (2003).

The ‘Dreiding’ models (Dreiding, 1959), used in chemistry to study conformations and flexibility of cycloalkenes and related molecules, are also physical realisations of N -loops. The atom components linked by peg-and-socket joints are rigid bodies linked by torsional revolute hinges; these bodies are free to rotate around the linking bond. For a given hybridisation of the carbon atom, the angle of intersection of the hinges is fixed, i.e., $\theta = \theta_T$ for sp^3 (where a saturated carbon centre participates in four single bonds),

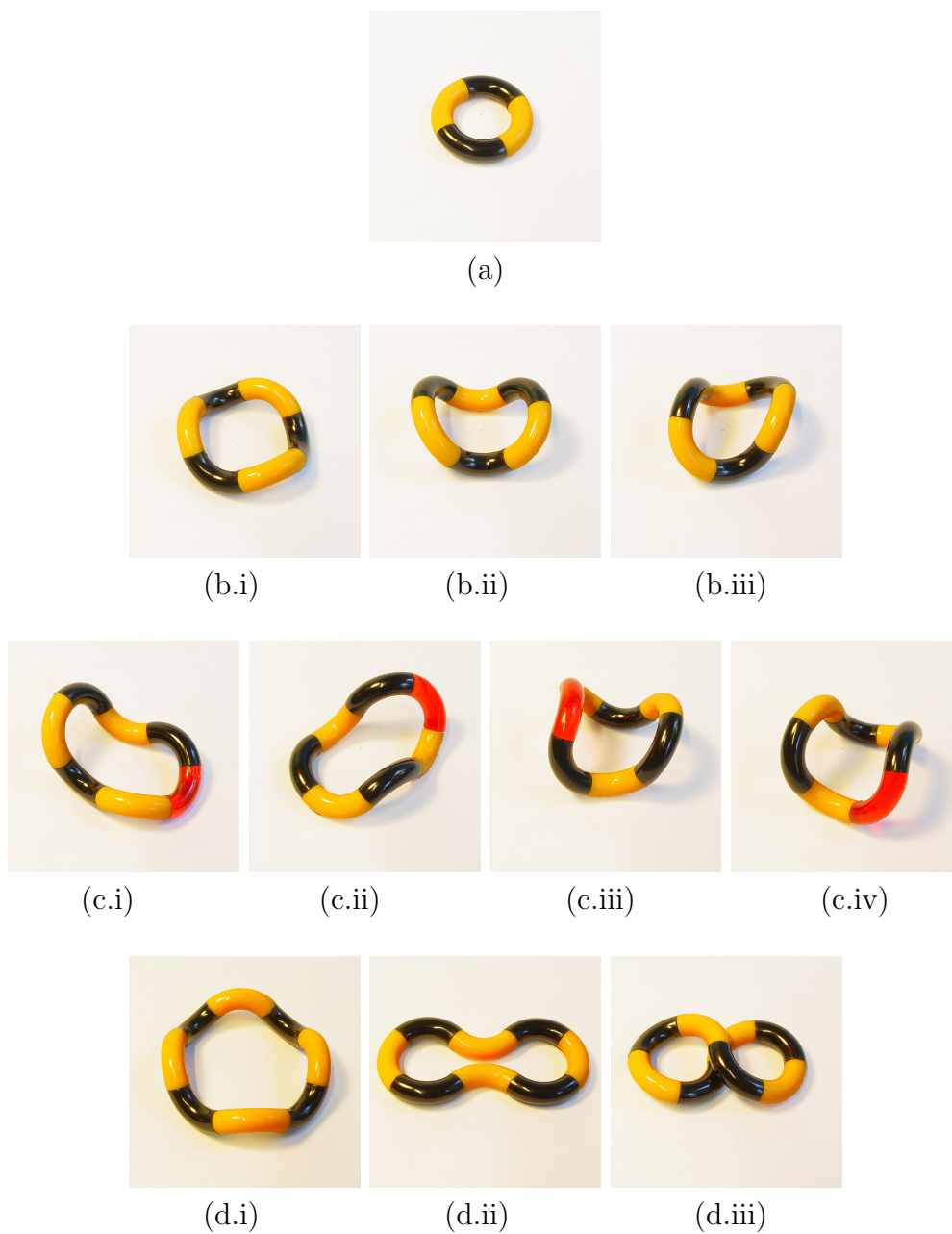


Figure 2: Conformations of Tangle models of N -loops, with $N = 4, 6, 7, 8$. Here $\theta = 90^\circ$ for all links.

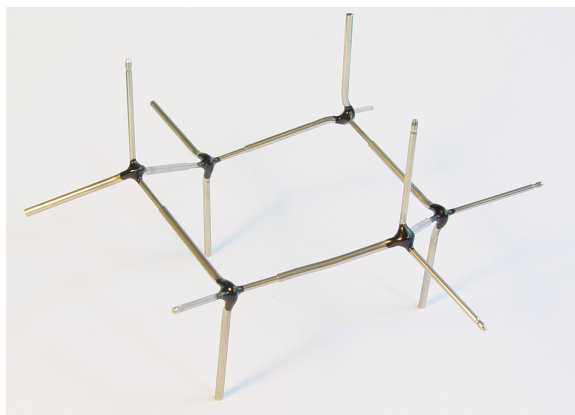
$\theta = 2\pi/3$ for sp^2 (where an unsaturated carbon centre participates in bonds to three neighbours). Figure 3 illustrates the use of Dreiding models for the well studied case of the cyclohexane ring (Eliel, 1962), where the models are 6-loops with $\theta = \theta_T$. The figure shows the three conformations identified in chemical nomenclature as chair, boat and twist-boat. The chair model, representing the low-energy molecular conformer, is rigid, whereas the boat and twist-boat models can be interconverted by rotation of hinges, following a one-parameter continuous path. (See, for example, Baker (1986), and the complete map of the conformation space given in a recent computational study, Porta et al. (2007).) Unlike the stiffer Tangle model, the chair Dreiding model can be ‘snapped through’ to the boat form by deformation of the components.

Even simpler models of N -loops are possible. Goldberg (1978) gives a net from which a paper model of Bricard’s (1897) flexible octahedron can be made, and as we show in Figure 4, this generates a corresponding non-regular 6-loop.

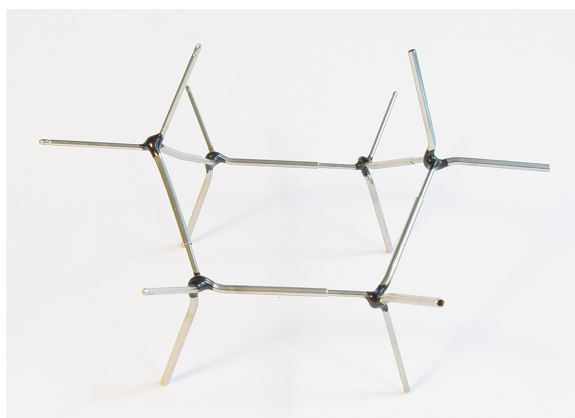
The concept of *mobility* is central to the analysis of the kinematic properties of all these models. The *mobility criterion* associated with the classic work of Kutzbach and Grübler (Hunt, 1978), is usually interpreted as a counting rule that quantifies the kinematic degrees of freedom of a system, and, in favourable cases, reveals the existence of mechanisms (freedoms) or states of self-stress (overconstraints). However, counting alone cannot distinguish, for example, between the rigid chair and non-rigid boat forms of the 6-loop. A key difference between the chair and boat forms is their point-group symmetry, and it turns out that symmetry considerations explain the difference in mobility. In the present paper, we cast the general symmetry-extended mobility criterion (Guest and Fowler, 2005) in a form suitable for the analysis of the kinematics of the N -loop, and use this to examine generically symmetric configurations for different values of N , strengthening the counting results, and rationalising the observed mobility in many cases.

2 Preliminary counting analysis

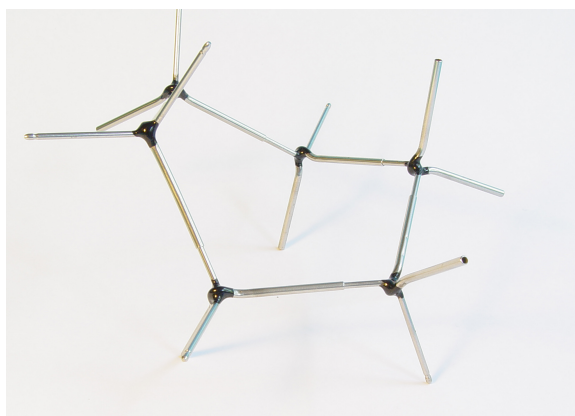
As a simple generic counting relationship for calculating the degrees of freedom of a mechanical linkage, the mobility criterion is a familiar concept in mechanism theory. In Hunt’s (1978) formulation, as extended by the present authors (Guest and Fowler, 2005), a mechanical linkage consisting of n bodies connected by g joints, where joint i permits f_i relative freedoms, has relative



(a)



(b)



(c)

Figure 3: Dreiding models of the cyclohexane ring in: (a) chair; (b) boat; and (c) twist-boat conformations.

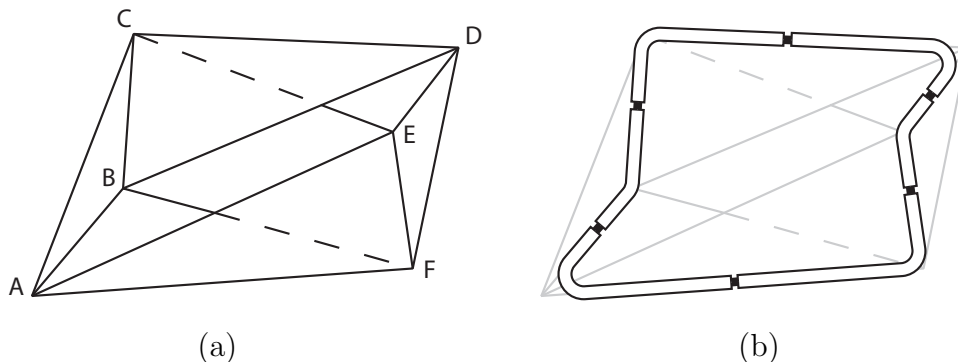


Figure 4: Flexibility of the Bricard octahedron. (a) Flattened form (after Goldberg, 1978) in which the intersecting faces BDF and ACE have been removed, thus allowing the rest of the structure to flex. (b) An equivalent planar non-regular 6-loop.

mobility:

$$m - s = 6(n - 1) - 6g + \sum_{i=1}^g f_i \quad (1)$$

where $m - s$ is the difference between the *mobility*, or number of mechanisms, m , and the number of independent states of self-stress, s . This equation counts the degrees of freedom by taking the difference between the relative body freedoms, of which there are $6(n - 1)$, and the constraints imposed by the joints, of which there are $\sum_{i=1}^g (6 - f_i)$.

For a loop of N components, the numbers of bodies and joints are equal, $n = g = N$, and each revolute hinge allows a single relative freedom, $f_i = 1$ for all i . Therefore,

$$m - s = 6(N - 1) - 6N + N = N - 6, \quad (2)$$

and the N -loop is guaranteed to have $m > 0$ mechanisms for all $N > 6$. For $N = 4$, the N -loop has at least two states of self-stress, and for $N = 5$ has at least one. For $N = 6$, the loop has equal numbers of mechanisms and states of self-stress, $m - s = 0$. For $N > 6$, each mechanism beyond the minimum count of $N - 6$ necessarily implies a corresponding extra state of self-stress.

Clearly, from the observations described in the introduction, this simple counting exercise has not captured all aspects of the mobility of an N -loop. For example, the 4-loop has in fact infinitesimal mobility, $m = 1$. The 6-loop has two forms, both with $m - s = 0$, but one is rigid ($m = s = 0$) and the other has finite mobility ($m = s = 1$). To gain further insight, we need a

symmetry-extended mobility criterion for N -loops that compares not only total numbers, but also symmetries, of the mechanisms and the states of self-stress.

3 A symmetry-extended mobility analysis

The extended mobility criterion (Guest and Fowler, 2005) relates the *representations* of the mechanisms and states of self-stress to those of various features of the structure. A representation $\Gamma(\text{object})$ describes the symmetry of a set of objects (which may be joints, bars, vectors or other local structural or dynamical motifs) in the relevant point group of the structure. $\Gamma(\text{object})$ collects the *characters* $\chi(S)$ of sets of objects, i.e., for each symmetry operation S , $\chi(S)$ is the trace of the matrix that relates the set before and after the application of S . For further details, see Bishop (1973).

In the language of representations, the extended mobility criterion for a collection of bodies can be written (Guest and Fowler, 2005)

$$\Gamma(m) - \Gamma(s) = \Gamma(\text{relative body freedoms}) - \Gamma(\text{hinge constraints}) \quad (3)$$

where $\Gamma(m)$ and $\Gamma(s)$ are respectively the representations of the mobility, and the states of self-stress. The *relative body freedoms* are the freedoms of all the bodies of the mechanical linkage, in the absence of connections, and taken relative to one body considered as a reference. The *hinge constraints* are those constraints imposed by hypothetical rigid joints, minus the actual freedoms at the joints. A rigid joint removes six freedoms, i.e., three relative rotations and three relative translations. In the present case, all joints are revolute hinges, each of which restores one relative rotational freedom about the line of the hinge joining a pair of bodies.

An alternative way of formulating the extended mobility criterion is to consider the relative mobility of the structure where all joints are fixed and rigid body motions are prevented, which we will call Γ_{fix} . To obtain $\Gamma(m) - \Gamma(s)$ we then restore the various hinge freedoms spanning $\Gamma(\text{hinge freedoms}) \equiv \Gamma_f$, and write

$$\Gamma(m) - \Gamma(s) = \Gamma_{\text{fix}} + \Gamma_f. \quad (4)$$

For a structure with all joints fixed, there can be no mechanisms, $\Gamma(m) = 0$, and it is apparent that Γ_{fix} is the negative of the representation of the states of self-stress of a completely rigid structure that has the same topology as the original linkage.

In describing the mobility of a general mechanical linkage, it is useful to define the linkage topology through what is often loosely called the *contact*

polyhedron C , a graph embedded in 3D space that has ‘vertices’ at bodies, and ‘edges’ through joints. The point group of this embedded graph is $G(C)$. (In fact, in the case of the N -loop, C reduces to a (non-planar) contact *polygon*, as each body is joined to exactly two others.) In terms of the properties of C , the symmetry-extended mobility rule of the general mechanical linkage is (Guest and Fowler, 2005)

$$\Gamma(m) - \Gamma(s) = (\Gamma_\sigma(v, C) - \Gamma_\parallel(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R) + \Gamma_f, \quad (5)$$

where $\Gamma_\sigma(v, C)$ is the *permutation representation* of the vertices of C (a permutation representation of a set has character $\chi(S)$ equal to the number of elements of the set left in place by the operation S), and where $\Gamma_\parallel(e, C)$ is the representation of a set of vectors along the edges of C . Γ_0 is the totally symmetric representation, with $\chi_0(S) = 1$ for all S , and Γ_T and Γ_R are the representations of rigid-body translations and rotations respectively. Γ_0 , Γ_T and Γ_R can be read off from standard point-group theory tables, e.g., Atkins et al. (1970), Altmann and Herzog (1994).

Substituting the formulation (4) in (5), we see that, for the general N -loop, Γ_{fix} is the 6-dimensional representation

$$\Gamma_{\text{fix}} = (\Gamma_\sigma(v, C) - \Gamma_\parallel(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R). \quad (6)$$

This expression can be simplified, as we will see below.

The other term in this approach to the calculation of mobility, Γ_f , which describes the set of hinge freedoms, is also associated with a structural representation of the contact polyhedron. The freedom of a revolute hinge, the axis of which is parallel to an edge of the contact polyhedron, is described in group-theoretical terms by Guest and Fowler (2005). Such a freedom has the nature of a local pseudo-scalar: if an operation S leaves a particular hinge unshifted, then the contribution to the overall character for the set of hinges is $+1$ for proper, and -1 for improper, operations S . Therefore, for the set of revolute hinges in an N -loop is

$$\Gamma_f = \Gamma_\sigma(e, C) \times \Gamma_\epsilon, \quad (7)$$

where $\Gamma_\sigma(e, C)$ is the permutation representation of the edges of C , and Γ_ϵ is the representation of a central pseudo-scalar, having character $\chi(S) = +1$ for proper, and -1 for improper S .

Substituting (7) into (5) gives a specific form of the mobility criterion applicable to an N -loop, the *loop equation*:

$$\Gamma(m) - \Gamma(s) = (\Gamma_\sigma(v, C) - \Gamma_\parallel(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R) + \Gamma_\sigma(e, C) \times \Gamma_\epsilon \quad (8)$$

This equation too can be greatly simplified by taking into account the properties of the different representations associated with C , as we will see below. It is convenient to split the discussion of Γ_{fix} (Section 3.1) and Γ_f (Section 3.2) before producing unified expressions for the mobility of the N -loop (Section 3.3).

3.1 States of self-stress in a ring structure

The highest point group symmetry $G(C)$ achievable by an $N(\theta)$ -loop is D_{Nh} (for the planar structure that exists when $\theta = 2\pi/N$). Any other conformation belongs to a subgroup of D_{Nh} , and results obtained in the higher group can be specialised to particular conformations using descent in symmetry or inspection of characters.

We use the standard D_{Nh} setting with the z -direction along the principal rotational axis. It is useful to present the odd $N = 2p + 1$ and even $N = 2p$ (both with $p > 0$) cases separately before writing the fully general formula.

3.1.1 N odd

For odd cycles, the edge and vertex representations are equal

$$(N \text{ odd}): \quad \Gamma_{\sigma}(e, C) = \Gamma_{\sigma}(v, C) \quad (9)$$

and, independently of the parity of N , the representation of a set of vectors along the edges of the cycle is

$$\Gamma_{\parallel}(e, C) = \Gamma(R_z) \times \Gamma_{\sigma}(e, C) \quad (10)$$

where $\Gamma(R_z)$ is the representation of the rotation about the principal axis.

The form of Equation 6 conceals a high degree of cancellation, which can be removed by considering an angular-momentum type expansion of the two vertex-related terms. In general, the odd cycle has contributions to $\Gamma_{\sigma}(v, C)$ from complete sets with axial angular momentum components 0 to $p = (N - 1)/2$.

$$(N \text{ odd}): \quad \Gamma_{\sigma}(v, C) = \Gamma_{\sigma}(e, C) = \Gamma_0 + \sum_{L=1}^p \Gamma_L = A'_1 + \sum_{L=1}^p E'_L. \quad (11)$$

where Γ_0 is the symmetry of the nodeless in-phase combination of all vertices and the notation Γ_L stands for the representation of the two independent combinations of vertices (or edges) with L angular nodal planes (corresponding to the set of two degenerate functions with components $\pm L$ of angular momentum about the principal axis).

As the vector representation $\Gamma_{\parallel}(e, C)$ arises by multiplication of $\Gamma_{\sigma}(e, C)$ with the one-dimensional representation $\Gamma(R_z) = A'_2$, the summation term is left unchanged, and $\Gamma_{\parallel}(e, C)$ and $\Gamma_{\sigma}(v, C)$ differ in only one term:

$$(N \text{ odd}): \quad \Gamma_{\parallel}(e, C) - \Gamma_{\sigma}(v, C) = \Gamma(R_z) - \Gamma_0 = A'_2 - A'_1. \quad (12)$$

Thus, for the odd- N loop, (6) becomes

$$(N \text{ odd}): \quad \Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -A'_1 - E'_1 - A''_1 - E''_1. \quad (13)$$

3.1.2 N even

For even cycles, edge and vertex representations are in general different. An even cycle is a *bipartite* graph, one in which vertices can be partitioned into two sets, such that no two members of a set are adjacent. Vertices of the cycle belong alternately to these ‘starred’ and ‘unstarred’ sets. The vertex representation for even N , as before, can be written as an expansion in angular momentum, but now also includes a final, non-degenerate, fully antisymmetric combination that has a change of sign between each adjacent pair of vertices. The symmetry of this special combination is the *alternating representation*, Γ_{\star} , which has character $\chi_{\star}(S) = +1$ for operations that preserve, and $\chi_{\star}(S) = -1$ for operations that swap, the starred and unstarred sets.

For even cycles, the difference between the vertex and edge permutation representations can be calculated from Γ_{\star} , as $\Gamma_{\sigma}(v, C)$ includes Γ_{\star} , but the edge representation includes $\Gamma_{\star} \times \Gamma(R_z)$, where Γ_{\star} and $\Gamma_{\star} \times \Gamma(R_z)$ form the two halves of the $L = p$ angular-momentum pair. The vertex and edge representations, for D_{ph} with p finite, are therefore

$$(N \text{ even}): \quad \Gamma_{\sigma}(v, C) = A_{1g} + \Gamma_{\star} + \sum_{L=1}^{p-1} E_{Lg/u}, \quad (14)$$

$$(N \text{ even}): \quad \Gamma_{\sigma}(e, C) = \Gamma_{\sigma}(v, C) - \Gamma_{\star} + \Gamma_{\star} \times \Gamma(R_z), \quad (15)$$

and the edge-vector representation (10) is

$$(N \text{ even}): \quad \Gamma_{\parallel}(e, C) = A_{2g} + \Gamma_{\star} + \sum_{L=1}^{p-1} E_{Lg/u}. \quad (16)$$

In (14) and (16), the notation means that $E_{Lg/u}$ has g symmetry for even L and u symmetry for odd L .

Thus, for the even- N loop, (6) becomes

$$(N \text{ even}): \quad \Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -A_{1g} - E_{1g} - A_{2u} - E_{1u}. \quad (17)$$

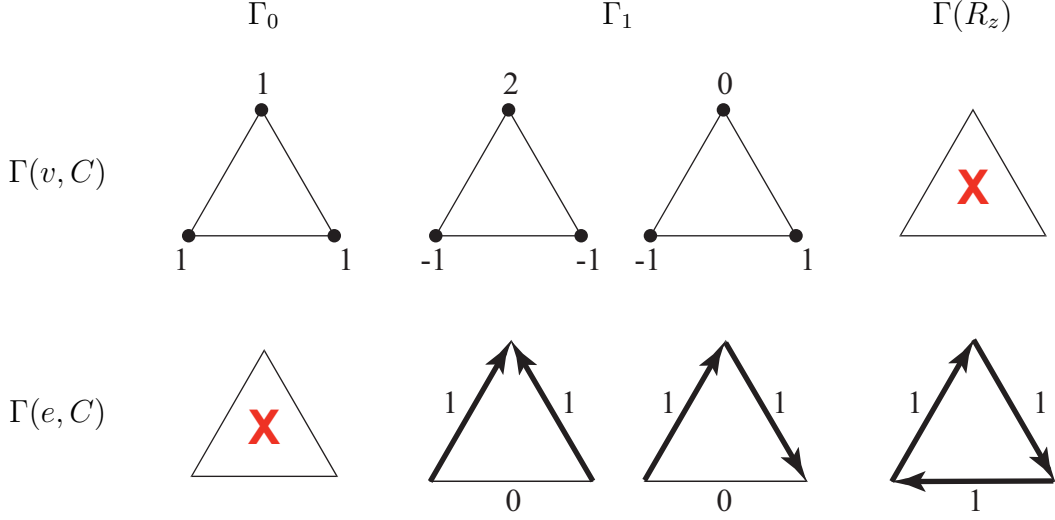


Figure 5: Correspondence between vertex- and edge-vector representations for cycles. Weights in the vertex combinations (top row) correspond to net flows into vertices in the edge-vector combinations (bottom row). Only one combination of each type is unmatched (**X**).

3.1.3 General formulation

Although the end results (13) and (17) appear superficially different because of the different notation for representations of D_{Nh} with odd and even N , they carry the same information, which is topological in character. The generic form for Γ_{fix} arises from the fact that, for any cycle, $\Gamma_{\parallel}(e, C)$ differs from $\Gamma_{\sigma}(v, C)$ only by substitution of $\Gamma(R_z)$ for Γ_0 . A cyclic array of arrows cannot be totally symmetric in D_{Nh} but it can achieve the symmetry of a rotation when all N arrows point in the same sense; a cyclic array of vertices can have a totally symmetric set of weights, but cannot have weights corresponding to rotation (Figure 5). Both odd- N and even- N cases are therefore represented by the general formula

$$\Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -\Gamma_0 - \Gamma_{\epsilon} - \Gamma(x, y) - \Gamma(R_x, R_y), \quad (18)$$

which can easily be specialised for any particular group. This can be done either by following the fate of the irreducible representations under descent in symmetry, or by using the characters $\chi(S)$ for the individual operations. Γ_{fix} has character zero under all improper operations (as it is proportional to $(\Gamma_T + \Gamma_R)$) and under proper operations it has $\chi_{\text{fix}}(E) = -6$, $\chi_{\text{fix}}(C_n) = -2 - 4 \cos \phi$, $\chi_{\text{fix}}(C'_2) = -2$.

The RHS of (18) is the (negative of the) generic symmetry description of the set of states of self-stress arising from the linking together of N bodies

in a cycle. This is a direct consequence of the toroidal topology of the linked bodies, and other rigid toroidal assemblies also have the same set of states of self-stress. The same symmetry has been derived for the states of self-stress of toroidal deltahedra using symmetry-extended Maxwell analysis (Fowler and Guest, 2002), and occurs as a contribution to the mobility equation for the toroidal rotating rings of tetrahedra (Fowler and Guest, 2005). The deltahedra are rigid and so have no term $\Gamma(m)$; compared to the N -loops, the rotating rings have a different mode of linkage and a different partial cancellation of $\Gamma(m)$ and $\Gamma(s)$. However, in all three cases, (18) appears as the symmetry description of the states of self-stress imposed by closure of a chain of bodies into a rigid torus.

3.2 Hinge freedoms for the N -loop

An angular-momentum-type expansion is also useful for the representation of the hinge freedoms, $\Gamma_f = \Gamma_\epsilon \times \Gamma_\sigma(e, C)$. In $D_{(2p+1)h}$, multiplication by $\Gamma_\epsilon = A_1''$ interconverts E_L' and E_L'' , and, from (11),

$$(N = 2p + 1): \quad \Gamma_f = \Gamma_\epsilon + \sum_{L=1}^p \Gamma_L \times \Gamma_\epsilon = A_1'' + \sum_{L=1}^p E_L'' \quad (19)$$

In D_{2ph} , multiplication by $\Gamma_\epsilon = A_{1u}$ interconverts E_{Lg} and E_{Lu} , and, from (15),

$$(N = 2p): \quad \Gamma_f = \Gamma_\epsilon + \Gamma_\star \times \Gamma(z) + \sum_{L=1}^{p-1} \Gamma_L \times \Gamma_\epsilon = A_{1u} + \Gamma_\star \times \Gamma(z) + \sum_{L=1}^{p-1} E_{Lu/g} \quad (20)$$

where the reversal of g/u subscripts in (20) means that odd L values now imply g , even L values imply u .

The general expression subsuming odd and even cases is therefore

$$\Gamma_f = \Gamma_\epsilon + [\Gamma_\star \times \Gamma(z)] + \sum_{L=1}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon \quad (21)$$

where the term in square brackets is understood to be omitted for odd N . This expression is easily specialised for any particular group: Γ_f has characters $\chi_f(E) = N = -\chi_f(\sigma_h)$, $\chi_f(C_n) = \chi_f(S_n) = \chi_f(i) = 0$, $\chi_f(\sigma_v) = e_v$, $\chi_f(C_2') = e_2$, where e_v , e_2 are the numbers of edges on the σ_v and C_2' symmetry elements, respectively.

3.3 Mobility of the N -loop

Substitution of (13),(19) and (17),(20) into the mobility criterion (8) leads to explicit expressions for the mobility of the N -loop:

$$(N = 2p + 1): \quad \Gamma(m) - \Gamma(s) = -A'_1 - E'_1 + \sum_{L=2}^p E''_L \quad (22)$$

$$(N = 2p): \quad \Gamma(m) - \Gamma(s) = A_{2u} \times \Gamma_\star - A_{1g} - E_{1u} + \sum_{L=2}^{p-1} E_{Lu/g} \quad (23)$$

$$(\text{all } N): \quad \Gamma(m) - \Gamma(s) = [\Gamma_\star \times \Gamma(z)] - \Gamma_0 - \Gamma(x, y) + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon \quad (24)$$

where $\Gamma(x, y)$ is the representation of the two translations in the plane perpendicular to the principal axis.

In equations such as (24) and (21), Γ_\star (defined only when N is even) depends on both the size of the N -loop and its setting within the point group. If we agree to fix the even- N -cycle in D_{Nh} so that C''_2 and σ_d symmetry elements each pass through vertices of the cycle, then Γ_\star has $\chi_\star(C''_2) = \chi_\star(\sigma_v) = -1$, $\chi_\star(C''_2) = \chi_\star(\sigma_d) = +1$, and is $\Gamma_\star = B_{2g}$ for $N = 4m$ and $\Gamma_\star = B_{2u}$ for $N = 4m + 2$. The term appearing in Γ_f and $\Gamma(m) - \Gamma(s)$ is then $\Gamma_\star \times \Gamma(z) = B_{1u}$ for $N = 4m$ and $\Gamma_\star \times \Gamma(z) = B_{1g}$ for $N = 4m + 2$.

Equation (24) is the generic symmetry description of the mobility arising from the linking together of N bodies in a cycle where the links are revolute hinges whose axes intersect. In many applications, the N -loop will be *regular*, i.e., it will be characterised by a single nearest-neighbour distance, and a constant intersection angle. However, (24) applies more generally, both for a regular object adopting a less symmetrical confirmation, and for an object with a more general distribution of distances and angles, when specialised to the appropriate point group.

4 Examples

In this section we will look at some general classes of conformations of N -loops, and examine the behaviour of small cases.

4.1 Planar conformations of N -loops

If the intersection angle θ is $\pi - 2\pi/N$, then a unique planar conformation is possible for a regular N -loop. We can use the present approach to derive a general formula for the mechanisms and states of self-stress in such conformations.

The group of the regular polygon is D_{Nh} . In the groups of this type there is no cancellation between the positive and negative terms of the RHS of (24), i.e., the non-degenerate representations $\Gamma_\star \times \Gamma(z)$, Γ_0 are not equal, and the degenerate $\Gamma(x, y)$ is not repeated by any of the terms under the summation sign. Hence we can be sure that the negative terms are included in the symmetry of the states of self stress and the positive terms in the symmetry of the mechanisms:

$$\Gamma(s) \supset \Gamma_0 + \Gamma(x, y) \quad (25)$$

$$\Gamma(m) \supset [\Gamma_\star \times \Gamma(z)] + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon \quad (26)$$

We can strengthen these inequality results by the following argument which fixes $\Gamma(s)$. Consider building up the cycle by introducing the N joints between the bodies one by one in a cyclic order. When $N - 1$ joints have been introduced, we have a chain of N bodies connected by $N - 1$ revolute hinges, each of which lies in the plane, and do far there are no states of self-stress. States of self-stress arise from possible misfits when connecting the final joint. No in-plane misalignment can be corrected by rotation of an in-plane hinge, but any out-of-plane misalignment can be corrected by appropriate hinge rotation. Thus, $s = 3$. The inequalities (25) and (26) become equalities, applicable for any N :

$$\Gamma(s) = \Gamma_0 + \Gamma(x, y) \quad (27)$$

$$\Gamma(m) = [\Gamma_\star \times \Gamma(z)] + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon \quad (28)$$

Note that the term containing Γ_\star is defined only for N even, and the summation over L is non-empty only for $N \geq 5$.

$N = 3$: The three-loop can exist only in a planar confirmation, and hence is generically rigid. Evaluation of $\Gamma(s)$ and $\Gamma(m)$ in D_{3h} leads straightforwardly in $\Gamma(s) = A'_1 + E'$ and $\Gamma(m) = 0$.

$N = 4$: In D_{4h} symmetry, with the convention that C_2'' and σ_d pass through a pair of vertices in the contact polyhedron, we have for the four-loop $\Gamma(m) - \Gamma(s) = B_{1u} - A_{1g} - E_u$, and hence $\Gamma(s) = A_{1g} + E_u$ and $\Gamma(m) = B_{1u}$. There is therefore an infinitesimal mechanism which may be blocked by the totally symmetric state of self-stress (Kangwai and Guest, 1999), and hence may not extend to a finite path.

$N \geq 5$: The 5-loop (D_{5h}) has $\Gamma(s) = A'_1 + E'_1$ and $\Gamma(m) = E''_2$. The 6-loop (D_{6h}) has $\Gamma(s) = A_{1g} + E_{1u}$ and $\Gamma(m) = B_{1g} + E_{2u}$. The series continues with $s = 3$ and $m = N - 3$, and the general forms of $\Gamma(s)$ and $\Gamma(m)$ in D_{Nh} are deducible from (23) and (22).

4.2 Crown conformations of N -loops

For even values of N , and intersection angles θ smaller than $\pi - 2\pi/N$, ‘crown’ conformations of $D_{(N/2)d}$ symmetry, in which the bodies lie alternately above and below the median plane, are possible. In $D_{(N/2)d}$, Γ_* is equal to $\Gamma(z)$ (B_2 when $N/2$ is even, A_{2u} when $N/2$ is odd), and the product $\Gamma(z) \times \Gamma_*$ is equal to Γ_0 . Degenerate representations in these groups obey

$$\Gamma_L \times \Gamma_\epsilon = \Gamma_{N/2-L} \quad (29)$$

and therefore the summation of $\Gamma_L \times \Gamma_\epsilon$ from $L = 2$ to $L = \lfloor (N-1)/2 \rfloor$ contains $\Gamma(x, y)$ for $N \geq 6$. Thus, both terms describing states of self-stress in (24) are cancelled out, leaving the following expressions for the mechanisms in the two distinct cases of even N .

$$(N = 4p + 2 \geq 6): \quad \Gamma(m) \supset \sum_{i=2}^{(N-2)/4} (E_{ig} + E_{iu}) \quad (30)$$

$$(N = 4p > 6): \quad \Gamma(m) \supset \sum_{i=2}^{(N-4)/2} E_i \quad (31)$$

$N = 4$: In the D_{2d} crown conformation of the 4-loop, $\Gamma(m) - \Gamma(s) = -\Gamma(x, y)$, indicating that $\Gamma(s)$ contains $\Gamma(x, y) = E$. The loop is generically rigid, and hence $s = 2$ and $\Gamma(s) = E$.

$N = 6$: In the D_{3d} crown conformation of the 6-loop, $\Gamma(m) - \Gamma(s) = 0$. This conformation is generically rigid with $m = s = 0$. The chair form of cyclohexane is a specific instance with $\theta = \theta_T$.

$N = 8$: In the D_{4d} crown conformation of the 8-loop, $\Gamma(m) - \Gamma(s) = E_2$. There is a degenerate pair of mechanisms, related by a rotation of $\pi/4$ about the principal axis. Each follows one of the pair of two-noded ($xy, x^2 - y^2$) harmonics. In each mechanism, one pair of bodies moves simultaneously outward, and another inward.

Mobilities for each crown conformation could also have been found by taking the mobility for the flat conformation, and making a descent in symmetry within the point-group chain $D_{Nh} \rightarrow D_{(N/2)d}$.

4.3 Special cases

Manipulation of models, as described in the introduction, reveals a number of conformations that do not fit into the previous classes.

$N = 6$ For $\theta = \pi/2$ the smallest special case occurs for $N = 6$, and is an analogue of the well-known ‘boat’ form of cyclohexane. Unlike the ‘chair’, this is a flexible conformation. Generically it retains only a C_2 axis through the ring centre, but can attain the higher symmetries C_{2v} and D_{2d} at special points along the path of the mechanism (Figure 2(b.ii,iii)).

In the generic C_2 conformation, $\Gamma(m) = \Gamma(s) = A - B$. At the D_{2h} conformation ($C_2(y)$ passing through two hinges), $\Gamma(m) = \Gamma(s) = B_1 - B_3$. At the C_{2v} conformation ($\sigma(y)$ passing through two hinges), $\Gamma(m) = \Gamma(s) = A_2 - B_2$. Hence there is a mechanism preserving a C_2 axis, and in the absence of a equisymmetric state of self-stress, this mechanism must extend to a finite one-dimensional path.

$N = 7$ The mobility count for generic conformations of the 7-loop implies the existence of at least one mechanism. Manipulation of the models with $\theta = \pi/2$ reveals two independent sets of non-interconverting conformations, analogues of the ‘boat’ and ‘chair’ of cycloheptane. Both are observed to be flexible, but generally with only the trivial symmetry C_1 . The maximum point groups, reached at special conformations, are C_s (boat and chair) and C_2 (‘twist’-boat and ‘twist’-chair). For all conformations, $\Gamma(m) - \Gamma(s)$ is a single irreducible representation. In the three accessible groups C_s, C_2, C_1 , this representation is, respectively, A'', B and A . This indicates at least one mechanism that acts to lower the symmetry at the high-symmetry points.

5 Conclusions

We have given a general description of the mobility of the N -loop. Given any particular geometric configuration of an N -loop, we can predict its mechanisms and states of self-stress in greater detail than would be possible by counting arguments alone, and in favourable cases, can give a complete symmetry description of the mechanisms and states of self-stress. To complete the picture, it would be interesting to determine for given N the ranges of θ for which conformations are realisable, and any induced partitioning of conformation space. For each realisable conformation, the symmetry machinery of the present approach can be applied. Techniques exist for numerical determination of realisability, and tracking of mechanisms in conformation space (Porta et al., 2007). Their application could give further insight into fields as diverse as chemical conformation analysis, and rigidity theory of engineering structures.

We note that it would be possible to extend the concept of N -loops to polycyclic and three dimensional cage topologies by allowing more than two hinged contacts per body. Such cases are equally amenable to a symmetry treatment of the type that we have described here. However, full polyhedra tend to be highly overconstrained.

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