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Fields Workshop on Rigidity and Symmetry 17 Oct 2011

Counting with symmetry: extended versions of mobility criteria

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Summary

Some self-justification

Chemistry, symmetry and the spherical shell

Euler's theorem and symmetry

The Cambridge approach

Maxwell's Rule and symmetry

Mobility Criterion and symmetry

Examples

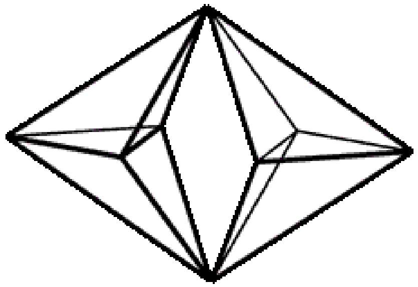
L'esprit de l'escalier

An extreme example ?

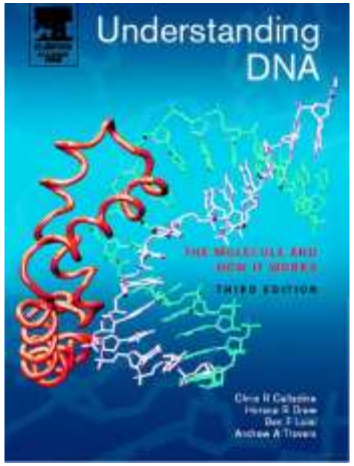
escalier. *Avoir l'esprit de l'escalier, par Honoré.*

http://www.larousse.fr/encyclopedie/data/images/1309806.jpg

“Why is a chemist interested in rigidity/symmetry?”



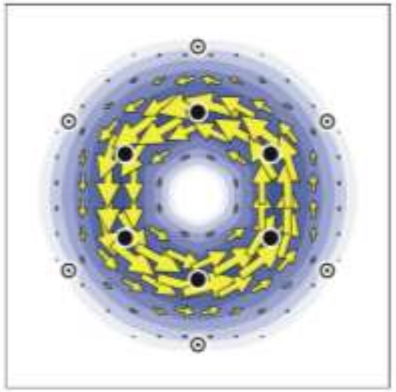
(Question from the floor to SDG:*
Calladine Retirement meeting, Cambridge, 2002)

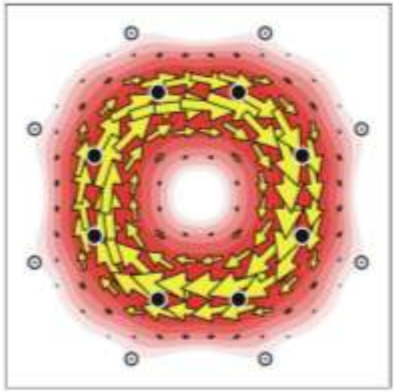


*Fowler, P.W. and Guest, S.D. (2002).
Symmetry Analysis of the double banana and related indeterminate structures,
New Approaches to Structural Mechanics, Shells and Biological Structures,
Drew H.R. and Pellegrino, S. eds., Kluwer, 91-101.

Chemists often count things:

electrons, orbitals, nodes, bonds, vibrations, quantum states …



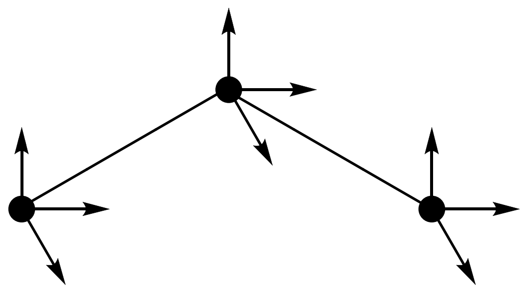


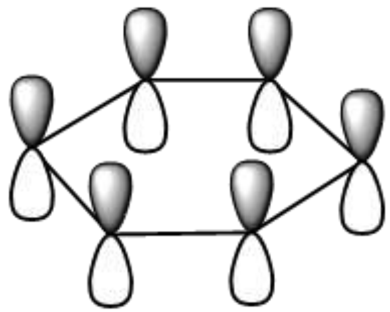
Huckel rule:	4N+2 π electrons	4N
Ipsocentric:	4 active electrons	2
	Aromatic	Anti-aromatic


4 LEGS GOOD
2 LEGS BAD

Chemistry, symmetry and the spherical shell

Molecules are often modelled as structures decorated with motifs that have some local symmetry.



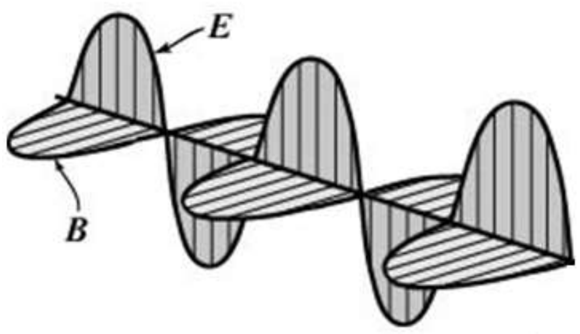


Clear analogies with engineering-scale structures decorated with states of self stress, mechanisms, …

Why is symmetry important in chemistry?

Experimental characterisation of
molecular shape, connectivity, bond strength, energy levels …
by spectroscopy

Absorption of radiation requires varying molecular dipole/polarisability



$\Rightarrow$ symmetry selection rules

e.g. IR / Raman Rule of Mutual Exclusion   O=C=O

The chemist's toolkit

point groups, character tables,
reduction of representations
descent in symmetry (the Jahn-Teller theorem)

C_{3v}	E	$2C_3$	$3\sigma_v$	
A_1	1	1	1	$z,\ x^2+y^2,\ z^2$
A_2	1	1	-1	R_z
E	2	-1	0	(x,y), (R_x, R_y), (xz, yz)

'Cultural' differences:

chemical training focused on rows of the character table, useful for e.g., $\Gamma(m)$- $\Gamma(s)$, but columns are useful too:

Connelly, R., Fowler, P.W., Guest, S.D., Schulze, B. and Whiteley, W.J. (2009)
When is a pin-jointed framework isostatic? Int Journal of Solids & Structures, 46, 762-773

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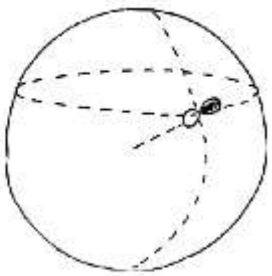
Representations of sets of objects
– decorations of points with scalar, vector, … functions

Spherical Shell Approach



Quinn, Redmond, McKiernan
(with some help from Frobenius)

Γ_σ Permutation representation of a set of points
Γ_π tangential vectors on those points
Γ_δ tangential quadrupoles …

CM Quinn, JG McKiernan, DB Redmond (1983) Inorg Chem 22, 2310
CM Quinn, JG McKiernan, DB Redmond (1984) J Chem Ed 61, 569, 572
PW Fowler, CM Quinn, Theor Chim Acta (1986) 70: 333

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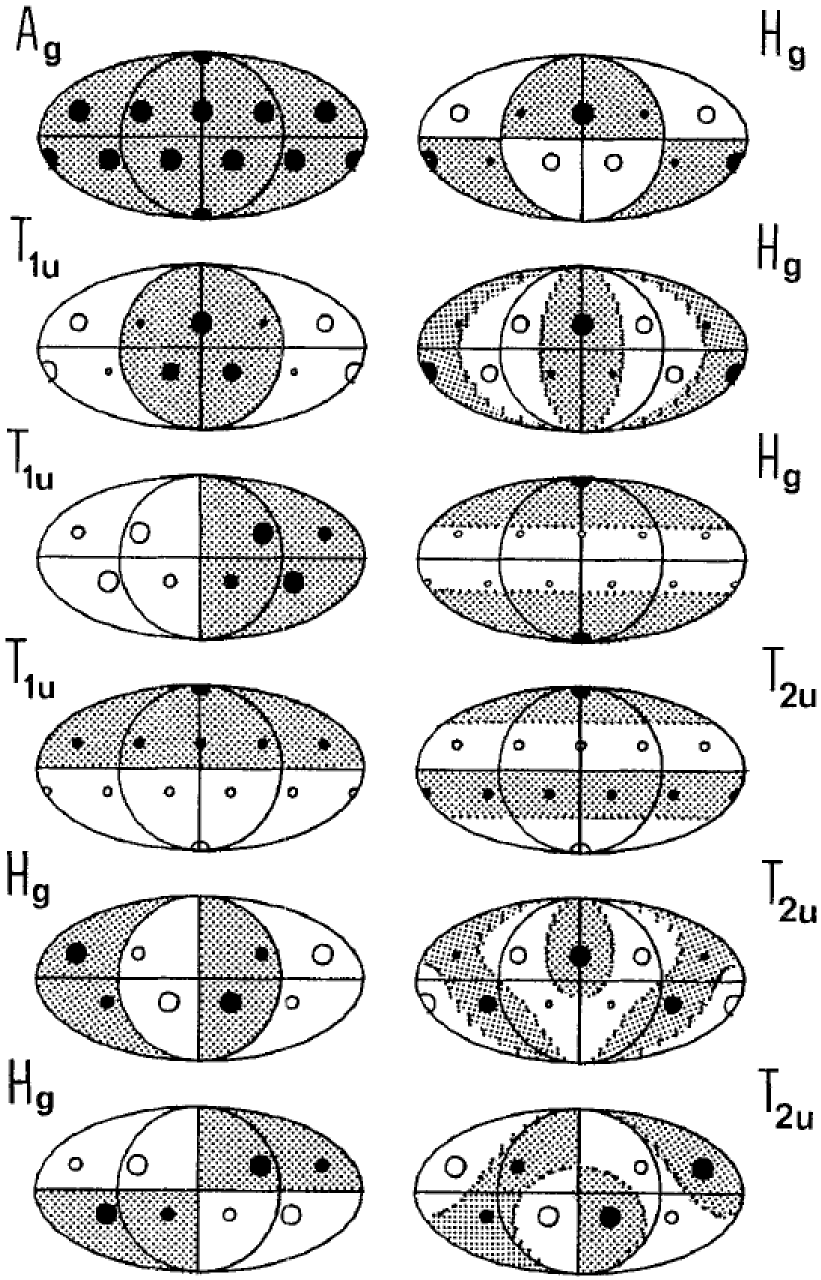
Icosahedron

σ combinations
of 12 vertices



Bootstrap theorems for spherical shell representations

$$\Gamma_\sigma$$

$$\Gamma_\pi = \Gamma_\sigma \times \Gamma_\mathrm{T} - \Gamma_\sigma$$

$$\Gamma_\delta = \Gamma_\pi \times \Gamma_\mathrm{T} - \Gamma_\pi - \Gamma_\sigma - \Gamma_\sigma \times \Gamma_\varepsilon$$

$$\Gamma_{\mathrm{L}+1} = \Gamma_\mathrm{L} \times \Gamma_\mathrm{T} - \Gamma_\mathrm{L} - \Gamma_{\mathrm{L}-1}$$

with Γ_ε the pseudoscalar representation

(and Γ_0 the totally symmetric representation)

$\Rightarrow$ Tensor Surface Harmonic theory of bonding in clusters

Obvious connection with vibrations

and engineering applications

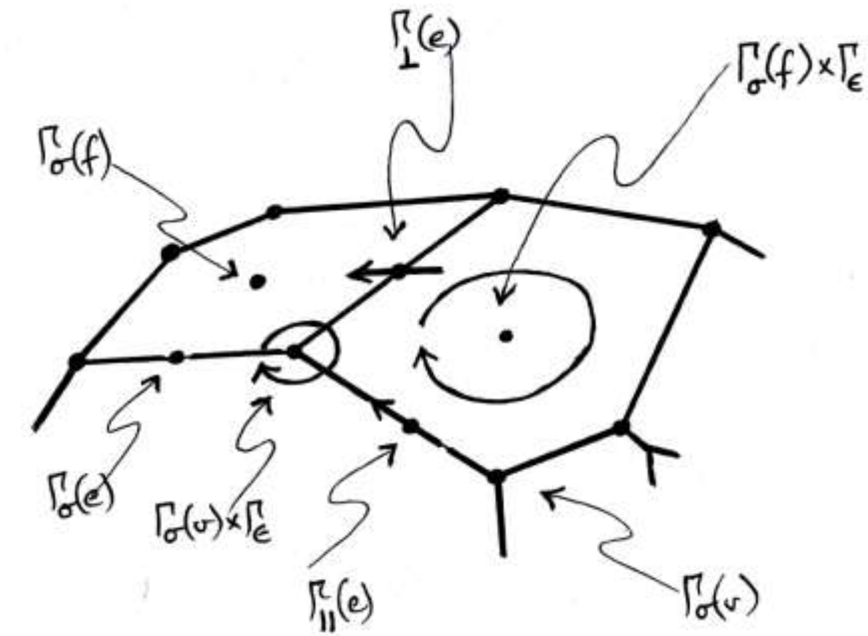
$$\Gamma_{3N} = \Gamma_\sigma + \Gamma_\pi$$

A symmetry extension of Euler's Theorem

$$v + f = e + 2$$

$$\Gamma_\sigma(v)\times\Gamma_\varepsilon + \Gamma_\sigma(f) = \Gamma_\perp(e) + \Gamma_0 + \Gamma_\varepsilon$$

$$\Gamma_\sigma(v) + \Gamma_\sigma(f)\times\Gamma_\varepsilon = \Gamma_\parallel(e) + \Gamma_0 + \Gamma_\varepsilon$$



A. Ceulemans and P.W. Fowler, Nature 353 (1991) 52-54
Extension of Euler's theorem to the symmetry properties of polyhedra

Proof by characters under the various types of operation

$$\Gamma_{\sigma}(v)\times\Gamma_{\varepsilon} + \Gamma_{\sigma}(f) = \Gamma_{\perp}(e) + \boxed{\Gamma_{0} + \Gamma_{\varepsilon}}$$

Two global motions on a sphere that cannot be generated by tangential motion across polyhedral edges:

radial breathing of all face centres

and

concerted rotation about all vertices

Vibrational representations

Deltahedra :

$$\Gamma_{\sigma}(v) \times \Gamma_{T} - \Gamma_{T} - \Gamma_{R} = \Gamma_{\sigma}(e)$$

Cubic Polyhedra :

$$\Gamma_{\sigma}(v) \times \Gamma_{T} = \Gamma_{\sigma}(e) + \Gamma_{\|}(e)$$

Applications:

vibrations of deltahedra: equisymmetric with stretches
cubic polyhedra: stretches and slides

bonding in deltahedra: uses only (*n*+1) electron pairs
cubic polyhedra: is edge precise (one pair per edge)

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Extensions : e.g. Toroidal Frameworks

$$v + f = e + 0$$

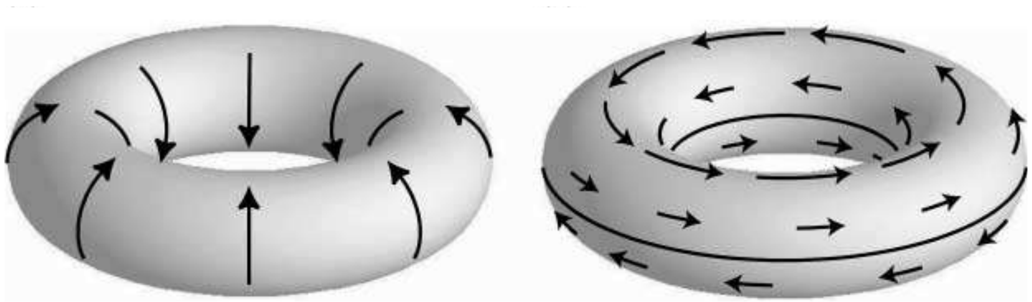
$$v + f + 2 = e + 2$$

$$\Gamma_\sigma(v)\times\Gamma_\varepsilon + \Gamma_\sigma(f) + \Gamma(R_z) + \Gamma(T_z) = \Gamma_\perp(e) + \Gamma_0 + \Gamma_\varepsilon$$

$$\Gamma_\sigma(f)\times\Gamma_\varepsilon + \Gamma_\sigma(v) + \Gamma(R_z) + \Gamma(T_z) = \Gamma_\parallel(e) + \Gamma_0 + \Gamma_\varepsilon$$

A. Ceulemans and P.W. Fowler, J. Chem. Soc. Faraday Trans. 91 (1995) 3089-3093
Symmetry extensions of Euler's theorem for polyhedral, toroidal and benzenoid molecules

Two global motions on a torus that can be generated by tangential motion across polyhedral edges but not by face breathing and local vertex rotations



$$\Gamma(T_z) \qquad \Gamma(R_z)$$

$$\Gamma_\sigma(v)\times\Gamma_\varepsilon \;+\; \Gamma_\sigma(f) \;\boxed{+\;\Gamma(T_z)\;+\;\Gamma(R_z)}\;=\Gamma_\perp(e)\;+\;\Gamma_0\;+\;\Gamma_\varepsilon$$

Meanwhile, back in Cambridge …

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Kangwai, R.D. (1997) PhD Thesis, University of Cambridge.
The analysis of symmetric structures using group representation theory.

Kangwai, R.D., Guest, S.D. and Pellegrino, S. (1999).
"Introduction to the Analysis of Symmetric Structures."
Computers & Structures **71**(2), 671-688.

Kangwai, R.D. and Guest, S.D. (1999).
"Detection of Finite Mechanisms in Symmetric Structures."
International Journal of Solids and Structures **36**, 5507-5527.

Kangwai, R.D. and Guest, S.D. (2000).
"Symmetry Adapted Equilibrium Matrices."
International Journal of Solids and Structures **37**, 1525-1548.

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Maxwell’s Rule and symmetry

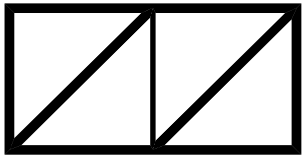
Maxwell’s Rule for pin-jointed frameworks

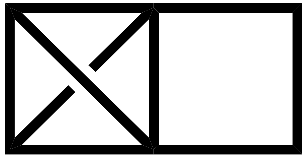
$$s - m = b - 3j + 6$$

$$\Gamma(s) - \Gamma(m) = \Gamma(b) - \Gamma(j) \times \Gamma_T + \Gamma_T + \Gamma_R \qquad \text{3D}$$

$$\Gamma(s) - \Gamma(m) = \Gamma(b) - \Gamma(j) \times \Gamma_{Tx,Ty} + \Gamma_{Tx,Ty} + \Gamma_{Rz} \qquad \text{2D}$$

J.C. Maxwell, On the calculation of the equilibrium and stiffness of frames
Phil. Mag, 27 (1864) 294–299
S. Pellegrino and C.R. Calladine, Matrix analysis of statically & kinematically indeterminate structures
Int. J. Solids Structures, 22 (1986) 409–428
PW Fowler and SD Guest, A symmetry extension of Maxwell’s Rule for rigidity of frames
Int J Solids Structures, 37 (2000) 1793-1804





C_2	E	C_2
$\Gamma(j)$	6	0
$\times\ \Gamma_T$	2	0
	12	0
$-\Gamma_T - \Gamma_R$	-3	1
	9	1
$-\Gamma(b)$	-9	-1
$\Gamma(m) - \Gamma(s)$	0	0

No mechanism/soss

C_s	E	σ	
$\Gamma(j)$	6	0	
$\times\ \Gamma_T$	2	0	
	12	0	
$-\Gamma_T - \Gamma_R$	-3	1	
	9	1	
$-\Gamma(b)$	-9	-3	
$\Gamma(m) - \Gamma(s)$	0	-2	$=-A' + A''$

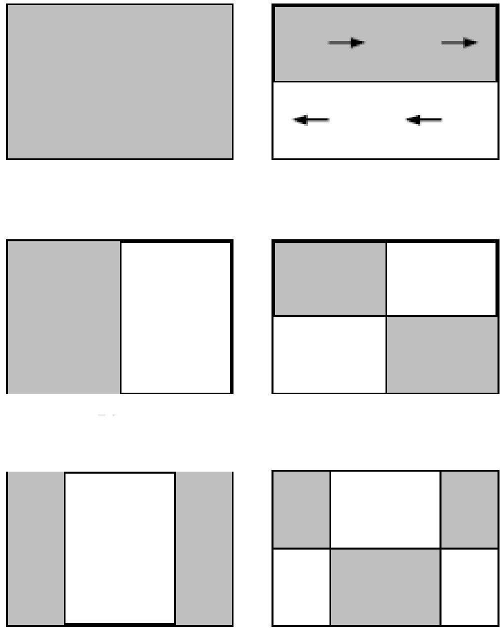
Antisymmetric mechanism and symmetric soss

Corollary (in combination with the Euler extension)

Maxwell (1870) : spherical deltahedron $s = m$

toroidal deltahedron $s - m \geq 6$

Every toroidal deltahedron has at least six soss, with symmetries related to translations and rotations



$$\Gamma(s) \geq (\Gamma_T + \Gamma_R) \times \Gamma_z$$

In the $D_{\infty h}$ parent group the six span

$$\Sigma_g^+ + \Sigma_g^- + \Pi_g + \Pi_u$$

P.W. Fowler and S.D. Guest, Int. J. Solids and Structures 39 (2002) 4385-4393
Symmetry and states of self stress in triangulated toroidal frames

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Another application : Danzerian rigidity

Spherical circle packing as a bar-joint assembly with uniform expansion allowed

$$f_D = 2\,j - b - 2$$

Danzer's 'almost conjecture' : f_D is positive $\Rightarrow$ packing is non-rigid

$$\Gamma(f_D) = \Gamma(m) - \Gamma(s) = \Gamma(j) \times (\Gamma_T - \Gamma_0) - \Gamma(b) - \Gamma_R + \Gamma_0$$

Our almost conjecture : $\Gamma(f_D)$ has a positive weight $\Rightarrow$ packing is non-rigid

'… new insight into ... historical development of improved circle packings … found through symmetry breaking from an initial … arrangement … '

P.W. Fowler, S.D. Guest, T. Tarnai : A symmetry treatment of Danzerian rigidity for circle packing, Proc. Roy. Soc. A, 464 (2008) 3237-3254.
L. Danzer, 1963, *Endliche Punktmengen auf der 2-Sphäre mit möglichts grossem Minimalabstand*. Habilitationsschrift, Universität Göttingen.

A symmetry-extended mobility rule

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The Grübler/Kurzbach criterion (extended à la Pellegrino/Calladine)

$$m - s = 6(n-1) - 6g + \sum_{l=1}^{g} f_l$$

n bodies
g joints
f_l relative freedoms of joint l

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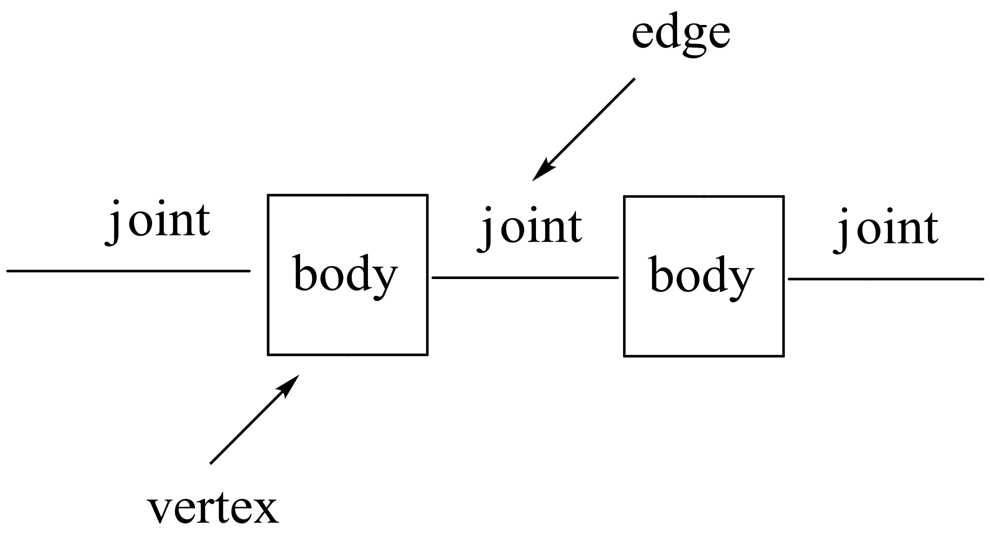
The symmetry version:

Define a contact “polyhedron”   C



Guest, S.D. and Fowler, P.W. (2005), "A symmetry-extended mobility rule."
Mechanism and Machine Theory. 40, 1002-1014

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

A B

A: $\Gamma(\text{relative body freedoms}) = \Gamma(\text{body freedoms}) - \Gamma(\text{rigid body motions})$

$$= \Gamma(v, C) \times (\Gamma_T + \Gamma_R) - \Gamma_T - \Gamma_R$$

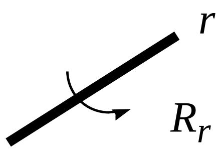
B: $\Gamma(\text{hinge constraints}) = \Gamma(\text{rigid joints}) - \Gamma(\text{joint freedoms})$

$$= \Gamma_{||}(e, C) \times (\Gamma_T + \Gamma_R) - \Gamma_{\text{freedoms}}$$

$$\Gamma(m) - \Gamma(s) = \left(\Gamma(v, C) - \Gamma_{||}(e, C) - \Gamma_0 \right) \times \left(\Gamma_T + \Gamma_R \right) + \Gamma_{freedoms}$$

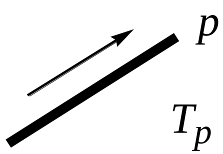
Freedoms of the joints

revolute



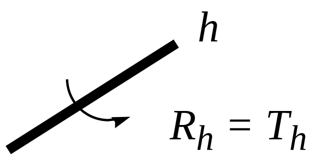
$\chi_{Rr}(S)\chi_{e||}(S)$

prismatic



$\chi_{Tp}(S)\chi_{e||}(S)$

screw



$\chi_{Rh}(S)\chi_{e||}(S)$

Examples: 4-bar linkage

D_{2d}: $\Gamma(m) - \Gamma(s) = -B_1 + B_2 - E$

(the unique) B_2 mechanism detected

Guest, S.D. and Fowler, P.W. (2005), Mechanism and Machine Theory. 40, 1002-1014

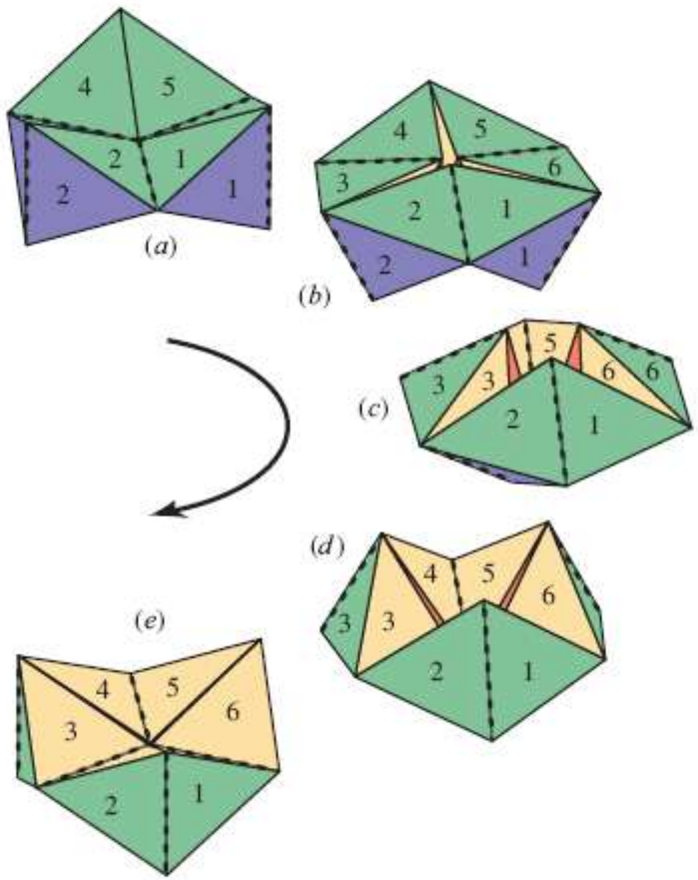
Rotating rings of tetrahedra

Mobility :

Even number of rigid tetrahedra hinged on opposite edges

Maxwell :

Tetrahedra as six spherical-jointed bars



Fowler, P.W. and Guest, S.D. (2005), "A symmetry analysis of mechanisms in rotating rings of tetrahedra." Proceedings of the Royal Society: Mathematical, Physical & Engineering Sciences. 461(2058), 1829-1846

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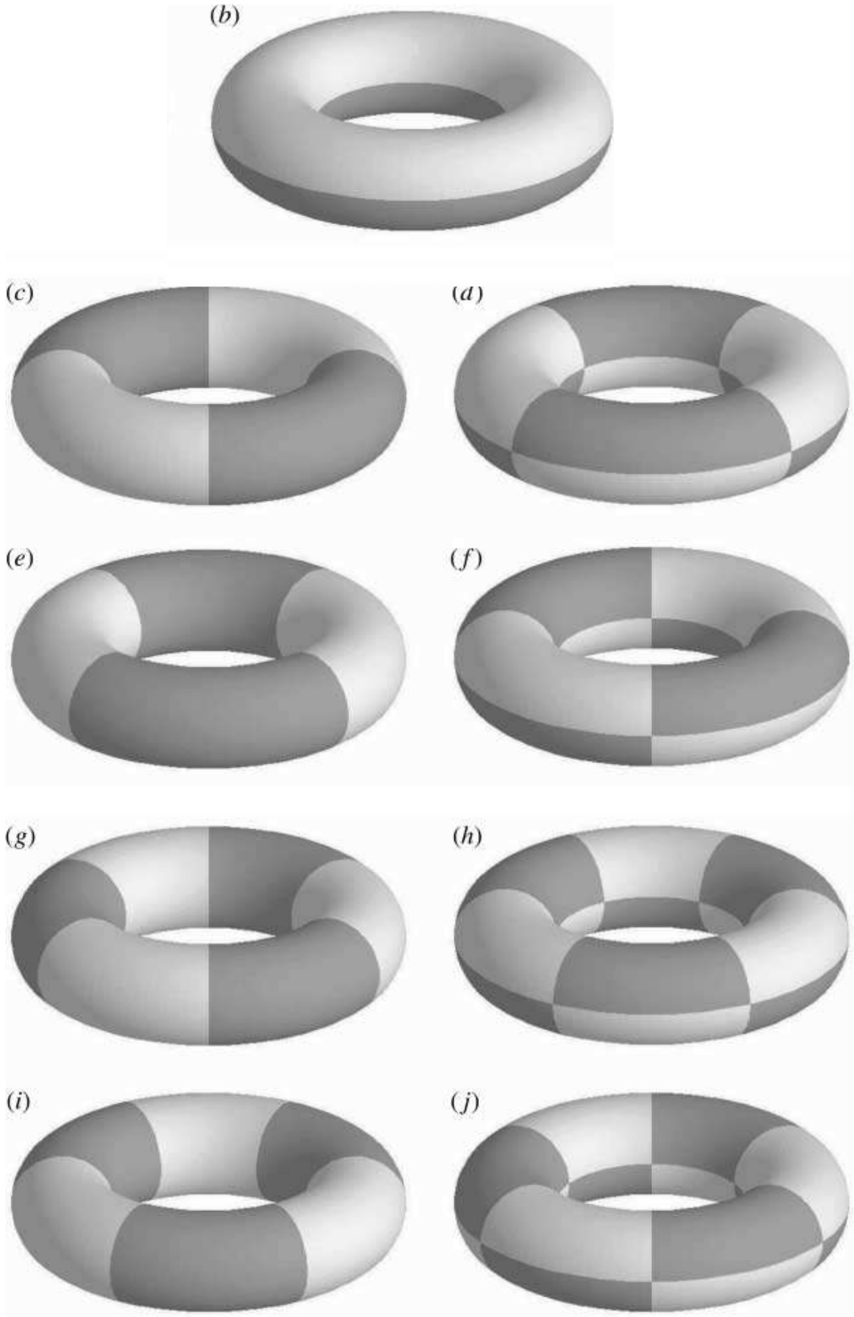
‘Angular momentum’ classification of mechanisms

N - 5 for *N* = 6, 8, 10 …



N-loops (Tangles)

$N = 4, 6, 7, 8$

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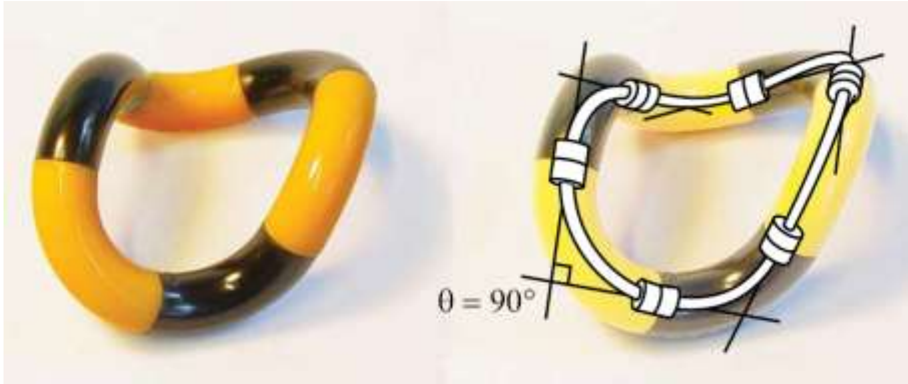
The model :



$$\Gamma(m) - \Gamma(s) = (\,\Gamma(v, C) - \Gamma_{||}(e, C) \ - \Gamma_0\,) \times (\,\Gamma_T + \Gamma_R\,) \ + \ \Gamma_{\text{freedoms}}$$

$$\Rightarrow \ \Gamma(m) - \Gamma(s) = (\,\Gamma(v, C) - \Gamma_{||}(e, C) \ - \Gamma_0\,) \times (\,\Gamma_T + \Gamma_R\,) \ + \ \Gamma\,(e, C) \times \Gamma_\varepsilon$$

Results (N > 5)

One soss of the pseudoscalar symmetry Γ_ε

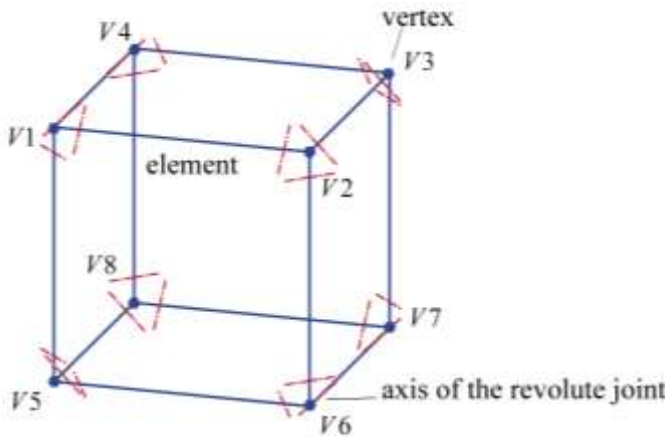
N - 5 mechanisms with symmetries defined by angular momentum expansion

$$\Gamma_z + (\Gamma_\Lambda \ - \Gamma_T - \Gamma_R\,)$$

Guest, S.D. and Fowler, P.W. (2010) "Mobility of *N*-loops: bodies cyclically connected by intersecting revolute hinges", Proceedings of the Royal Society: Mathematical, Physical & Engineering Sciences, 466, 63-77.

Our latest application :

The Hoberman Switch-Pitch and Polyhedral Variants*



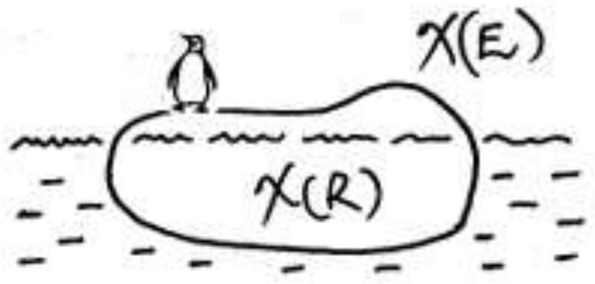
Counting: m-s = -6 : no indication of a mechanism

Symmetry: $\Gamma(m) - \Gamma(s) = A_{2u} - A_{1u} - T_{1g} - T_{1u}$

*Chen, Guest, Fowler, Feng, Wei, Ding (In preparation,2011)

Conclusions

A counting rule is often the tip of a symmetry iceberg.



Counting by classes of symmetry operation or by representations gives access to more rules

Refines rules that are necessary but not sufficient (e.g., Maxwell)

Gives a symmetry criterion for finiteness of mechanisms

For excess quantities (e.g., $m-s$) often identifies the key mechanism

High symmetry points can reveal ‘generic’ finite motions

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The next challenge: Symmetry, rigidity and periodicity

Rigidity of periodic and symmetric structures in nature and engineering

The Kavli Royal Society Centre
Chicheley Hall, Buckinghamshire

23rd and 24th February, 2012

Organisers: Simon Guest, Patrick Fowler, Stephen Power

http://royalsociety.org/events/Rigidity-of-periodic-and-symmetric-structures/