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Some Helical Structures Generated by Reflexions*

A. C. Hurley

Division of Chemical Physics, CSIRO,
P.O. Box 160, Clayton, Vic. 3168.

Abstract

There has recently been a revival of interest in the helical structure built up as a column of face-sharing tetrahedra, because of possible applications in structural crystallography (Nelson 1983). This structure and its analogues in spaces of different dimensions are investigated here. It is shown that the only crystallographic cases are the structures in one- and two-dimensional space. For three and higher dimensional space the structures are all non-crystallographic. For the physically important case of three dimensions, this result is implicit in an early discussion by Coxeter (1969). Results obtained here include explicit formulae for the positions of all vertices of the simplexes for dimensions $n = 1$–4 and a demonstration that, for arbitrary n, the ratio of the translation component of the screw to the edge of the simplex is $\{6/n(n+1)(n+2)\}^{\frac{1}{2}}$.

1. Introduction

A regular tetrahedron with vertices A, B, C, D may be imbedded in the unit cube in such a way that the coordinates of all the vertices are integers. If now one of the vertices, say A, is reflected through the opposite face BCD of the tetrahedron, a new vertex A′ is formed and a new tetrahedron BCDA′. The coordinates of the new vertex A′ are rational functions of the coordinates of A, B, C, D and are, therefore, all rational numbers. By reflecting the vertices B, C, D, A′, B′, ... in turn, one generates an infinite structure for which Buckminster Fuller has coined the convenient name *tetrahelix*. Its handedness depends upon the order in which the reflexions are effected; an odd permutation of A, B, C, D reverses the handedness. From the above argument it is clear that all vertices of the infinite tetrahelix have rational coordinates. Furthermore, as is easily shown, the edge length of the regular tetrahedron is a lower bound to the separation of any two vertices. From these properties we might hope that the infinite tetrahelix would form a crystallographic structure with some, perhaps very large, unit cell. We show that this is not the case, although the corresponding structures in one and two dimensions are crystallographic. We also consider the four-dimensional and the general n-dimensional cases.†

* Dedicated to Dr A. McL. Mathieson on the occasion of his 65th birthday.

† We note that n here corresponds to $n-1$ in the treatment by Coxeter (1985).

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2. Coordinate System and Representation of Reflexions

The starting tetrahedron is chosen to have vertices A, B, C, D with position vectors

$$\boldsymbol{a}_0 = (0,0,0), \qquad \boldsymbol{b}_0 = (0,1,1), \qquad \boldsymbol{c}_0 = (1,0,1), \qquad \boldsymbol{d}_0 = (1,1,0). \tag{1}$$

In discussing the helical structures, $\boldsymbol{a}_0$, $\boldsymbol{b}_0$, $\boldsymbol{c}_0$, $\boldsymbol{d}_0$ will be used as basic vectors, rather than the cartesian axes. This leads to a simpler treatment which is, moreover, readily transferred to spaces of higher and lower dimensionality.

If we reflect vertex A through the opposite face BCD, we arrive at a new vertex A′ with position vector

$$\boldsymbol{a}_1 = -\boldsymbol{a}_0 + \tfrac{2}{3}(\boldsymbol{b}_0 + \boldsymbol{c}_0 + \boldsymbol{d}_0). \tag{2}$$

Since the other vertices B, C, D of the new tetrahedron are unaltered by the reflexion, the transformation from the original tetrahedron to the new tetrahedron may be expressed by the transfer matrix $\mathbf{M}_a$, which satisfies

$$\begin{bmatrix} \boldsymbol{a}_1 \\ \boldsymbol{b}_0 \\ \boldsymbol{c}_0 \\ \boldsymbol{d}_0 \end{bmatrix} = \mathbf{M}_a \begin{bmatrix} \boldsymbol{a}_0 \\ \boldsymbol{b}_0 \\ \boldsymbol{c}_0 \\ \boldsymbol{d}_0 \end{bmatrix} = \begin{bmatrix} -1, & \frac{2}{3}, & \frac{2}{3}, & \frac{2}{3} \\ 0, & 1, & 0, & 0 \\ 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \end{bmatrix} \begin{bmatrix} \boldsymbol{a}_0 \\ \boldsymbol{b}_0 \\ \boldsymbol{c}_0 \\ \boldsymbol{d}_0 \end{bmatrix}. \tag{3}$$

Similarly we define transfer matrices $\mathbf{M}_b, \mathbf{M}_c, \mathbf{M}_d$ for reflexion of the vertices B, C, D respectively. They are given by the equations

$$\mathbf{M}_b = \begin{bmatrix} 1, & 0, & 0, & 0 \\ \frac{2}{3}, & -1, & \frac{2}{3}, & \frac{2}{3} \\ 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \end{bmatrix}, \qquad \mathbf{M}_c = \begin{bmatrix} 1, & 0, & 0, & 0 \\ 0, & 1, & 0, & 0 \\ \frac{2}{3}, & \frac{2}{3}, & -1, & \frac{2}{3} \\ 0, & 0, & 0, & 1 \end{bmatrix}, \tag{4a, b}$$

$$\mathbf{M}_d = \begin{bmatrix} 1, & 0, & 0, & 0 \\ 0, & 1, & 0, & 0 \\ 0, & 0, & 1, & 0 \\ \frac{2}{3}, & \frac{2}{3}, & \frac{2}{3}, & -1 \end{bmatrix}. \tag{4c}$$

3. Transfer Matrix

The process of successively reflecting the vertices A, B, C, D through their opposite faces effects a transformation of position vectors by a transfer matrix **M** which is given by the matrix product

$$\mathbf{M} = \mathbf{M}_\mathrm{d}\mathbf{M}_\mathrm{c}\mathbf{M}_\mathrm{b}\mathbf{M}_\mathrm{a} = \frac{1}{81}\begin{bmatrix} -81, & 54, & 54, & 54 \\ -54, & -45, & 90, & 90 \\ -90, & 6, & 15, & 150 \\ -150, & 10, & 106, & 115 \end{bmatrix}. \tag{5}$$

This transfer matrix leads directly from the position vectors $\boldsymbol{a}_0, \boldsymbol{b}_0, \boldsymbol{c}_0, \boldsymbol{d}_0$ to the position vectors $\boldsymbol{a}_1, \boldsymbol{b}_1, \boldsymbol{c}_1, \boldsymbol{d}_1$ of the next four points on the tetrahelix:

$$\begin{bmatrix} \boldsymbol{a}_1 \\ \boldsymbol{b}_1 \\ \boldsymbol{c}_1 \\ \boldsymbol{d}_1 \end{bmatrix} = \mathbf{M}\begin{bmatrix} \boldsymbol{a}_0 \\ \boldsymbol{b}_0 \\ \boldsymbol{c}_0 \\ \boldsymbol{d}_0 \end{bmatrix}. \tag{6}$$

If we iterate the above procedure, we find that the position vector of every vertex

$$(\boldsymbol{a}_0\, \boldsymbol{b}_0\, \boldsymbol{c}_0\, \boldsymbol{d}_0\, \boldsymbol{a}_1\, \boldsymbol{b}_1\, \boldsymbol{c}_1\, \boldsymbol{d}_1\, \boldsymbol{a}_2\, \boldsymbol{b}_2 \ldots \boldsymbol{a}_t\, \boldsymbol{b}_t\, \boldsymbol{c}_t\, \boldsymbol{d}_t \ldots)$$

may be obtained from $\boldsymbol{a}_0, \boldsymbol{b}_0, \boldsymbol{c}_0, \boldsymbol{d}_0$ and the matrix $\mathbf{M}$. Explicitly, we have

$$\begin{bmatrix} \boldsymbol{a}_t \\ \boldsymbol{b}_t \\ \boldsymbol{c}_t \\ \boldsymbol{d}_t \end{bmatrix} = \mathbf{M}^t\begin{bmatrix} \boldsymbol{a}_0 \\ \boldsymbol{b}_0 \\ \boldsymbol{c}_0 \\ \boldsymbol{d}_0 \end{bmatrix}. \tag{7}$$

In principle, equations (5) and (7) provide a complete description of the tetrahelix. However, as is evident from equation (5), the matrix $\mathbf{M}^t$ becomes extremely cumbersome even for moderate values of t. A much more transparent description is obtained by using the characteristic equation for the matrix $\mathbf{M}$, namely

$$\det(\lambda\mathbf{E}-\mathbf{M}) = \lambda^4 - \tfrac{4}{81}\lambda^3 - \tfrac{154}{81}\lambda^2 - \tfrac{4}{81}\lambda + 1 = 0, \tag{8}$$

with roots

$$1, \quad 1, \quad \alpha = (-79+8\sqrt{-5})/81, \quad \overline{\alpha}, \tag{9}$$

in order to transform $\mathbf{M}$ to its Jordan canonical form, which is found to be

$$\mathbf{S}^{-1}\mathbf{M}\mathbf{S} = \mathbf{M}_\mathrm{J} = \begin{bmatrix} 1, & 0, & 0, & 0 \\ 1, & 1, & 0, & 0 \\ 0, & 0, & \alpha, & 0 \\ 0, & 0, & 0, & \overline{\alpha} \end{bmatrix}. \tag{10}$$

In this form the calculation of $\mathbf{M}^t$ is trivial:

$$\mathbf{S}^{-1}\mathbf{M}^t\mathbf{S} = \mathbf{M}_J^t = \begin{bmatrix} 1, & 0, & 0, & 0 \\ t, & 1, & 0, & 0 \\ 0, & 0, & \alpha^t, & 0 \\ 0, & 0, & 0, & \overline{\alpha}^t \end{bmatrix}. \tag{11}$$

This program involving the explicit calculation of $\mathbf{S}$ has been carried through to obtain explicit coordinates for all points on the tetrahelix. The details will not be given in view of the simpler treatment in later sections. It is already apparent, however, from equations (8) and (10), that the structure cannot be crystallographic. From equations (10) and (11) it is apparent that the repeated eigenvalue 1 corresponds to the translational component of a screw, the remaining simple eigenvalues giving the rotational component. For the tetrahelix to be crystallographic, some power of $\mathbf{M}_J$ must be a pure translation. Hence all eigenvalues must be roots of unity. But since all roots of unity are algebraic integers, this would imply that the monic characteristic equation (8) has only integral coefficients; this is clearly not the case.

Change in Handedness

We have seen that the transfer matrix

$$\mathbf{M} = \mathbf{M}_d \mathbf{M}_c \mathbf{M}_b \mathbf{M}_a \tag{12}$$

describes a screw motion (equation 10). Since the individual transfer matrices satisfy the relations

$$\mathbf{M}_a^2 = \mathbf{M}_b^2 = \mathbf{M}_c^2 = \mathbf{M}_d^2 = \mathbf{E}, \tag{13}$$

$$\det \mathbf{M}_a = \det \mathbf{M}_b = \det \mathbf{M}_c = \det \mathbf{M}_d = -1, \tag{14}$$

it is easy to see that any odd permutation of the factors in $\mathbf{M}$ leads to a transfer matrix $\mathbf{M}'$ whose handedness is opposite to that of $\mathbf{M}$. For example, we have

$$\mathbf{M}' = \mathbf{M}_a \mathbf{M}_d \mathbf{M}_c \mathbf{M}_b = \mathbf{M}_a . \mathbf{M} . \mathbf{M}_a^{-1} \tag{15}$$

and, since det $\mathbf{M}_a$ has the value -1, the transformation (15) involves a change in handedness.

4. A Simpler Description

The treatment outlined above has been carried through for $n \leqslant 5$ but leads to severe complications in the case of general n, where the transfer matrix $\mathbf{M}$ involves the product of n elementary reflexions. A much simpler description is obtained if, after each reflexion, the position vectors $\boldsymbol{a}_i$ are relabelled in such a way that the entire helix results from the iteration of a single transformation $\mathbf{T}$. Thus in the three-dimensional case, if we relabel the position vectors $\boldsymbol{a}_0\, \boldsymbol{b}_0\, \boldsymbol{c}_0\, \boldsymbol{d}_0\, \boldsymbol{a}_1\, \boldsymbol{b}_1 \ldots$ in a single sequence

$$x_0\, x_1\, x_2\, x_3\, x_4\, x_5 \ldots, \tag{16}$$

the successive tetrahedra in the helical structure are

$$\begin{matrix} x_0\, x_1\, x_2\, x_3\, x_4 & & \\ & x_1\, x_2\, x_3\, x_4\, x_5 & \\ & & x_2 \ldots, \end{matrix} \tag{17}$$

and all of the transfer matrices assume the same form **T**. Thus, we write

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \mathbf{T} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0, & 1, & 0, & 0 \\ 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \\ -1, & \frac{2}{3}, & \frac{2}{3}, & \frac{2}{3} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}, \tag{18}$$

and for $s > 0$

$$\begin{bmatrix} x_s \\ x_{s+1} \\ x_{s+2} \\ x_{s+3} \end{bmatrix} = \mathbf{T} \begin{bmatrix} x_{s-1} \\ x_s \\ x_{s+1} \\ x_{s+2} \end{bmatrix} = \mathbf{T}^s \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}. \tag{19}$$

If we evaluate the first few powers of **T** we find

$$\mathbf{T}^2 = \begin{bmatrix} 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \\ -1, & \frac{2}{3}, & \frac{2}{3}, & \frac{2}{3} \\ \frac{2}{3}, & \frac{5}{9}, & \frac{10}{9}, & \frac{10}{9} \end{bmatrix}, \qquad \mathbf{T}^3 = \begin{bmatrix} 0, & 0, & 0, & 1 \\ -1, & \frac{2}{3}, & \frac{2}{3}, & \frac{2}{3} \\ \frac{2}{3}, & \frac{5}{9}, & \frac{10}{9}, & \frac{10}{9} \\ \frac{10}{9}, & \frac{2}{27}, & \frac{5}{27}, & \frac{50}{27} \end{bmatrix}, \tag{20}$$

$$\mathbf{T}^4 = \frac{1}{81} \begin{bmatrix} -81, & 54, & 54, & 54 \\ -54, & -45, & 90, & 90 \\ -90, & 6, & 15, & 150 \\ -150, & 10, & 106, & 105 \end{bmatrix}. \tag{21}$$

Comparing equations (21) and (5), we see that

$$\mathbf{T}^4 = \mathbf{M} = \mathbf{M}_\mathrm{d}\, \mathbf{M}_\mathrm{c}\, \mathbf{M}_\mathrm{b}\, \mathbf{M}_\mathrm{a}, \tag{22}$$

showing that the present treatment is consistent with that in terms of the elementary reflexions.

From equation (19) we see that the position vector x_s of a general vertex of the helix is given in terms of the basic vectors x_0, x_1, x_2 and x_3 by just the first row of the matrix $\mathbf{T}^s$:

$$x_s = \sum_{i=1}^{4} T_{1i}^s\, x_{i-1}. \tag{23}$$

Furthermore, from equation (20) we see that for $s = 0$–3 the first row of $\mathbf{T}^s$ has a very simple form:

$$T^s_{1i} = \delta_{i,s+1} \qquad (s = 0\text{–}3). \tag{24}$$

As we shall see in the next section these relations, which generalize easily to the n-dimensional case, give a very simple evaluation of the position vector of a general vertex x_s on the n-dimensional helix.

5. The n-Dimensional Case

At this point it is convenient to go over to the n-dimensional case. The key formulae of Section 4 are readily generalized, enabling us to treat all dimensionalities simultaneously. The basic vectors are now the vertices of a regular simplex in n dimensions:

$$x_0,\ x_1,\ \ldots,\ x_n \tag{25}$$

and the transfer matrix $\mathbf{T}$ is given by

$$\begin{bmatrix} x_s \\ x_{s+1} \\ x_{s+2} \\ \vdots \\ x_{s+n} \end{bmatrix} = \mathbf{T} \begin{bmatrix} x_{s-1} \\ x_s \\ \vdots \\ \vdots \\ x_{s+n-1} \end{bmatrix} = \mathbf{T}^s \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} \qquad (s > 0), \tag{26}$$

with

$$\mathbf{T} = \begin{bmatrix} 0, & 1, & 0, & \ldots, & 0 \\ 0, & 0, & 1, & & \vdots \\ \vdots, & & & & 0 \\ 0, & & & 0, & 1 \\ -1, & 2/n, & \ldots, & 2/n, & 2/n \end{bmatrix}. \tag{27}$$

Equations (23) and (24) immediately generalize to

$$x_s = \sum_{i=1}^{n+1} T^s_{1i}\, x_{i-1} \qquad (s > 0), \tag{28}$$

$$T^p_{1i} = \delta_{i,p+1} \qquad (p = 0, 1, \ldots, n). \tag{29}$$

From the form of the matrix $\mathbf{T}$ of equation (27) it is clear that the characteristic polynomial $f(\lambda)$ is also the minimal polynomial and that the characteristic equation is

$$\det(\lambda\mathbf{E}-\mathbf{T}) \equiv f(\lambda) = \lambda^{n+1} - (2/n)(\lambda^n + \lambda^{n-1} \ldots + \lambda) + 1 = 0. \tag{30}$$

Since the coefficient $2/n$ in equation (30) is an integer only if n has the values 1 or

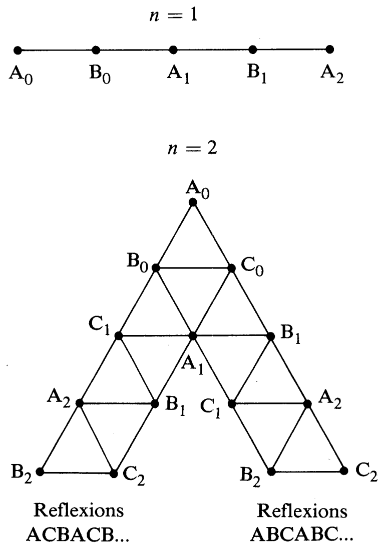

Fig. 1. Crystallographic cases for $n = 1$ and 2.

2, the structure can be crystallographic only in these cases (cf. Section 3). That the cases $n = 1, 2$ are in fact crystallographic is evident from Fig. 1, which illustrates these simple cases. We note that in both cases there is only one infinite structure (to within translation and rotation), rather than the left-handed and right-handed non-crystallographic forms for $n \geqslant 3$.

6. Position Vector of the General Vertex

The strategy we adopt is to express a general power of $\mathbf{T}$ in terms of the first n powers by means of the resolvent, and then extract x_s from the simple relations (28) and (29).

The characteristic equation (30) has the factor $(\lambda-1)^2$. Defining polynomials $g(\lambda)$ and $h(\lambda)$ by the equations

$$\det(\lambda\mathbf{E}-\mathbf{T}) = f(\lambda) = (\lambda-1)\, g(\lambda) = (\lambda-1)^2\, h(\lambda), \tag{31}$$

we find that

$$f(\lambda) = \lambda^{n+1} + 1 - \frac{2}{n} \sum_{p=0}^{n-1} \lambda^{n-p}, \tag{32}$$

$$g(\lambda) = \sum_{p=0}^{n} \left(1 - \frac{2p}{n}\right) \lambda^{n-p}, \tag{33}$$

$$h(\lambda) = \sum_{p=1}^{n} \frac{p(n-p+1)}{n} \lambda^{n-p}. \tag{34}$$

All other roots of the characteristic equation (30) are simple. They are all of modulus unity and, for odd n, all appear in complex conjugate pairs; for even n the final root $\alpha_{n-1} = -1$ appears singly. Thus, in both cases, we can express the complete set of roots as

$$\{1, 1, \alpha_1 = \exp(2\mathrm{i}\,\theta_1),\ \alpha_2 = \exp(-2\mathrm{i}\,\theta_1),\ \ldots,\ \alpha_{n-1}\}. \tag{35}$$

In evaluating a general analytic function $F(\mathbf{T})$ of the transfer matrix, we follow the notation and terminology of Zadeh and Desoer (1963) which should be consulted for further details.

By the matrix analogue of Cauchy's theorem we write

$$F(\mathbf{T}) = \frac{1}{2\pi\mathrm{i}} \oint_{\mathrm{C}} F(\lambda)\,(\lambda\mathbf{E}-\mathbf{T})^{-1}\,\mathrm{d}\lambda, \tag{36}$$

where the contour C encloses all the singularities given by the roots (35) of the characteristic equation. There is a contribution to (36) from each of the roots. The contribution from the repeated root $(\lambda-1)^2$ may be evaluated in the form

$$F(1,\mathbf{T}) = \{\mathbf{E}\,F(1) + (\mathbf{T}-\mathbf{E})\,F'(1)\}\,\mathbf{E}_1, \tag{37}$$

where

$$\mathbf{E}_1 = \phi_1(\mathbf{T}) = \{h(1)\,h(\mathbf{T}) - h'(1)\,g(\mathbf{T})\}/\{h(1)\}^2. \tag{38}$$

The numerical factors in equation (38) are readily evaluated using the explicit expression (34) for $h(\lambda)$. We find

$$h(1) = \tfrac{1}{6}(n+1)(n+2), \tag{39}$$

$$h'(1) = \tfrac{1}{12}(n^2-1)(n+2), \tag{40}$$

so that the contribution (37) may be expressed as

$$F(1,\mathbf{T}) = \frac{\{6F'(1) - 3(n-1)\,F(1)\}\,g(\mathbf{T}) + 6F(1)\,h(\mathbf{T})}{(n+1)(n+2)}. \tag{41}$$

All other roots of the characteristic equation are simple. Their contribution may be evaluated using Sylvester's interpolation formula (Zadeh and Desoer 1963) which gives, for root α_i,

$$F(\alpha_i,\mathbf{T}) = \frac{F(\alpha_i)\,(\mathbf{T}-\mathbf{E})^2}{(\alpha_i-1)^2} \prod_{j=1\neq i}^{n-1} \frac{\mathbf{T}-\alpha_j\mathbf{E}}{\alpha_i-\alpha_j}. \tag{42}$$

Unlike the contribution (41), the contributions (42) (except for $\alpha_i = -1$) can be evaluated explicitly only by solving the characteristic equation (30). This is a simple matter for $n \leqslant 4$, since only quadratic equations are involved. In the general case, Coxeter (1985) shows that if one puts $\lambda = \exp(2\mathrm{i}\,\theta)$ as in (35), equation (30) is equivalent to the equation

$$\tan\{(n+1)\theta\} = (n+1)\tan\theta, \tag{43}$$

which provides an efficient route to numerical solutions.

Assembling the contributions (41) and (42) and specializing to the function $F(\mathbf{T}) = \mathbf{T}^s$, we obtain for all $s \geqslant 0$

$$\mathbf{T}^s = \frac{\{6s-3(n-1)\}\, g(\mathbf{T})+6h(\mathbf{T})}{(n+1)(n+2)} + \sum_{i=1}^{n-1} \frac{\alpha_i^s(\mathbf{T}-\mathbf{E})^2}{(\alpha_i-1)^2} \prod_{j=1\neq i}^{n-1} \frac{\mathbf{T}-\alpha_j\mathbf{E}}{\alpha_i-\alpha_j}. \tag{44}$$

In order to obtain an explicit formula for x_s we re-express equation (44) as a sum over powers of $\mathbf{T}$:

$$\mathbf{T}^s = \sum_{p=0}^{n} C_p(n)\,\mathbf{T}^p, \tag{45}$$

where the coefficients are known functions of s and the roots α_i. Substituting the expression (45) into equation (28) and using the simple form (29) for the first row of T^p, we obtain

$$x_s = \sum_{p=0}^{n} \sum_{i=1}^{n+1} C_p(n)\, T_{1i}^p\, x_{i-1}$$

$$= \sum_{p=0}^{n} \sum_{i=1}^{n+1} C_p(n)\, \delta_{i,p+1}\, x_{i-1},$$

so that

$$x_s = \sum_{p=0}^{n} C_p(n)\, x_p. \tag{46}$$

From equation (46) we see that the coefficients $C_p(n)$ defined in equation (45) are the coordinates of the general vertex in the basis provided by the position vectors of the original simplex. In the Appendix we list values of the coefficients $C_p(n)$ for $n \leqslant 4$.

In the three-dimensional case we may express the final results in terms of the cartesian axes of equation (1). Denoting unit vectors along the x, y and z axes by $\boldsymbol{i}$, $\boldsymbol{j}$ and $\boldsymbol{k}$ respectively and using the results in the Appendix we find that the position vector of the sth vertex of the tetrahelix is given by

$$\begin{aligned} x_s =& (\boldsymbol{i}/50)\{20s-5+5s\cos(2s\theta)-7\sqrt{5}\sin(2s\theta)\} \\ &+(\boldsymbol{j}/50)\{10+10s-10\cos(2s\theta)+14\sqrt{5}\sin(2s\theta)\} \\ &+(\boldsymbol{k}/50)\{35-35\cos(2s\theta)-5\sqrt{5}\sin(2s\theta)\}, \end{aligned} \tag{47}$$

where $2\theta = \arccos(-\tfrac{2}{3})$.

Rearranging terms in equation (47), we find

$$x_s = v_0 + v_1\, s + v_c \cos(2s\theta) + v_s \sin(2s\theta) \tag{48a}$$

with

$$v_0 = \tfrac{1}{50}(-5i+10j+35k), \tag{48b}$$

$$v_1 = \tfrac{1}{50}(20i+10j), \tag{48c}$$

$$v_c = \tfrac{1}{50}(5i-10j-35k), \tag{48d}$$

$$v_s = \tfrac{1}{50}(-7\sqrt{5}\, i+14\sqrt{5}\, j-5\sqrt{5}\, k). \tag{48e}$$

Here v_0 (i.e. $-v_c$) represents the origin of the centre of the bounding cylinder, v_1 gives the translation at each step ($\Delta s = 1$), while v_c and v_s give the rotational components. We note that

$$v_1 . v_c = v_1 . v_s = v_s . v_c = 0$$

and the radius r_s of the bounding cylinder of the screw is

$$r_s = |v_c| = |v_s| = \tfrac{3}{10}\sqrt{6}.$$

7. Translational Component of the Elementary Screw Operation

Of special interest is the term in equation (44) which is proportional to s. This term may be evaluated without solving the characteristic equation and yields the translational component τ of the elementary screw operation. From equations (44)–(46) and the expansion (33) of $g(\lambda)$ we find

$$\begin{aligned} \tau &= \frac{6}{(n+1)(n+2)} \sum_{p=0}^{n} (1-2p/n)x_{n-p} \\ &= \frac{6}{n(n+1)(n+2)} \sum_{p=0}^{[\frac{1}{2}n]} (n-2p)(x_{n-p}-x_p). \end{aligned} \tag{49}$$

Since any two edges of a regular simplex which do not intersect are mutually orthogonal, because they belong to a regular tetrahedron, we can write

$$(x_{n-p}-x_p).(x_{n-q}-x_q) = \delta_{pq}\, l^2 \qquad (p,\, q < [\tfrac{1}{2}n]), \tag{50}$$

where l is the length of an edge of the simplex. Hence from equation (49) we have

$$\begin{aligned} \tau . \tau &= \left(\frac{6}{n(n+1)(n+2)}\right)^2 \sum_{p=0}^{[\frac{1}{2}n]} (n-2p)^2 l^2 \\ &= \tfrac{1}{2} l^2 \left(\frac{6}{n(n+1)(n+2)}\right)^2 \sum_{p=0}^{n} (n-2p)^2 . \end{aligned} \tag{51}$$

Equation (51) reduces to

$$\tau / l = \{6/n(n+1)(n+2)\}^{\frac{1}{2}}, \tag{52}$$

a surprisingly simple result. For $n = 1$–4 it yields, respectively, 1, $\frac{1}{2}$, $1/\surd 10$, $1/2\surd 5$, in agreement with the values in the Appendix, and the results of Coxeter (1985). Similarly, for even dimensionality n (i.e. $n = 2r$), we may evaluate the vector coefficient $\boldsymbol{\rho}$ of the reflexion term $(-1)^s$ in equation (44) as an explicit function of r. Using the fact that, for any regular simplex, adjacent edges meet at an angle of $\frac{1}{3}\pi$, we find for the magnitude $\rho = |\boldsymbol{\rho}|$ the relation

$$\rho/l = \{(2r+1)/8r(r+1)\}^{\frac{1}{2}}. \tag{53}$$

Comparing equations (52) and (53) we see that as r increases, ρ decreases much more slowly than τ. For $n = 2$ and 4, equation (53) yields, respectively, $\surd 3/4$ and $\surd 15/12$, which are readily seen to be consistent with values in the Appendix. For the vector coefficients of the remaining terms α_i^s ($i = 1, 2, \ldots$) in equation (44) which give the rotational components of the n-dimensional helix, we cannot expect simple general formulae such as (52) and (53). These terms require the solution of the characteristic equation (30) or, equivalently, of Coxeter's (1985) equation (43). For large n the equations will not be solvable in terms of radicals. This has been verified explicitly for the sextic equation

$$7x^6 - 210x^5 + 1365x^4 - 2860x^3 + 2145x^2 - 546x + 35 = 0,$$

which may be derived from equation (43) with $n = 14$ by expanding $\tan(n+1)\theta$ in powers of $\tan\theta$ (Coxeter 1985) and putting $x = \tan^2\theta$.

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Appendix

The roots of the characteristic equations are listed here, together with the coefficients $C_p(n)$ [equations (45) and (46)] for dimensionality $n = 1$–4.

For $n = 1$, with roots 1, 1, the coefficients are

$$C_0(1) = 1-s, \qquad C_1(1) = s.$$

For $n = 2$, with roots $1, 1, -1$, the coefficients are

$$C_0(2) = \tfrac{1}{4}\{3-2s+(-1)^s\},$$

$$C_1(2) = \tfrac{1}{2}\{1-(-1)^s\},$$

$$C_2(2) = \tfrac{1}{4}\{2s-1+(-1)^s\}.$$

For $n = 3$, with roots 1, 1, $\alpha = \exp(2\mathrm{i}\,\theta)$, $\bar{\alpha}$, where

$$\alpha = \tfrac{1}{3}(-2+\mathrm{i}\sqrt{5}), \qquad 2\theta = \arccos(-\tfrac{2}{3}) = 131{\cdot}81°,$$

the coefficients are

$$C_0(3) = \tfrac{1}{10}(-3s+6)+\tfrac{1}{50}(20\cos 2s\theta-\sqrt{5}\sin 2s\theta),$$

$$C_1(3) = \tfrac{1}{10}(-s+5)+\tfrac{1}{50}(-25\cos 2s\theta+8\sqrt{5}\sin 2s\theta),$$

$$C_2(3) = \tfrac{1}{10}(s+2)+\tfrac{1}{50}(-10\cos 2s\theta-13\sqrt{5}\sin 2s\theta),$$

$$C_3(3) = \tfrac{1}{10}(3s-3)+\tfrac{1}{50}(15\cos 2s\theta+6\sqrt{5}\sin 2s\theta).$$

For $n = 4$, with roots 1, 1, $\beta = \exp(2\mathrm{i}\,\phi)$, $\bar{\beta}$, -1, where

$$\beta = \tfrac{1}{4}(-1+\mathrm{i}\sqrt{15}), \qquad 2\phi = \arccos(-\tfrac{1}{4}) = 104{\cdot}48°,$$

the coefficients are

$$C_0(4) = \tfrac{1}{10}(-2s+5)+\tfrac{1}{6}(-1)^s+\tfrac{1}{75}(25\cos 2s\phi-\sqrt{15}\sin 2s\phi),$$

$$C_1(4) = \tfrac{1}{20}(-2s+9)-\tfrac{1}{4}(-1)^s-\tfrac{1}{75}(15\cos 2s\phi-7\sqrt{15}\sin 2s\phi),$$

$$C_2(4) = \tfrac{3}{10}+\tfrac{1}{6}(-1)^s-\tfrac{1}{75}(35\cos 2s\phi+5\sqrt{15}\sin 2s\phi),$$

$$C_3(4) = \tfrac{1}{20}(2s+1)-\tfrac{1}{4}(-1)^s+\tfrac{1}{75}(15\cos 2s\phi-7\sqrt{15}\sin 2s\phi),$$

$$C_4(4) = \tfrac{1}{10}(2s-3)+\tfrac{1}{6}(-1)^s+\tfrac{1}{75}(10\cos 2s\phi+6\sqrt{15}\sin 2s\phi).$$

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