Tiling the Plane with Chiral Tiles and the Space with Chiral Tetrahedra

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Abstract

We report on some methods used to detect chirality discriminations in Biomacromolecules. The transcription of Euclidean distances from data obtained in 2 dimensions to the 3-dimensional molecular architecture is shown to be discarded by another interpretation based on elementary foundations of non-euclidean geometry.

Keywords: Steiner Ratio, chirality discrimination, upper bound.

1 Introduction

In a foregoing work [1] , we have reported on some development related to the problem of upsurge of chirality in macromolecular structures. The usual idea is that a macromolecule can be considered chiral as related to other macromolecule if the mirror image of the first is non-superposable on the other. Usually we say that a macrostructure has chiral properties if their constituents (monomers) are themselves chiral. After the discovery of the structure of carbon atom with its valencies directed towards the vertices of a regular tetrahedron, this monomeric property become apparent. It is known that we can identify two molecular structures by considering the bonding of four different chemical groups to the central carbon atom. These molecular structures are chiral to each other.

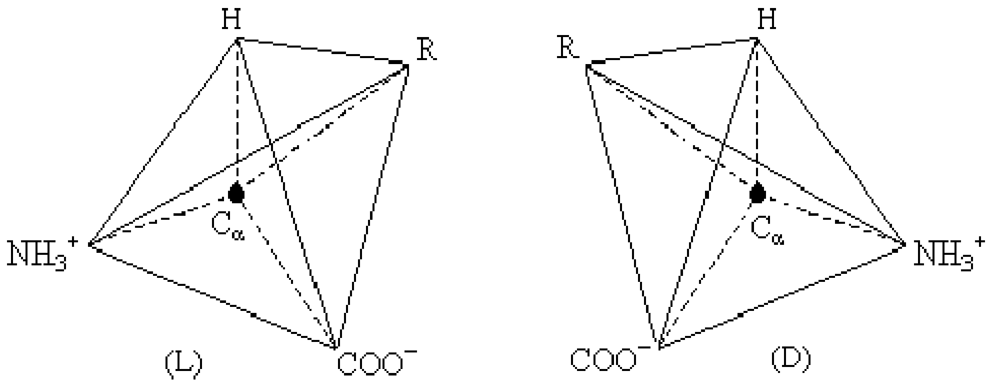

Figure 1: The levogirous (L) and dextrogirous (D) forms (isomers) of each aminoacid. R stands for the specific side chain.

Actually, the structures above cannot be represented by regular tetrahedra, due to different eletronegativity of the four groups attached to the α-carbon in the centre. We think that the chirality property has a deeper significance than that based in the structures above. It is so-to-say related to the geometric notion of distance which is necessary for length measure in the macromolecular structure. It is also a property of the 3-dimensional space inside a biomacromolecule. Let us suppose for fixing the ideas, a method for building tetrahedra. If these are supposed regular, we divide an equilateral triangle into four equilateral triangles, or

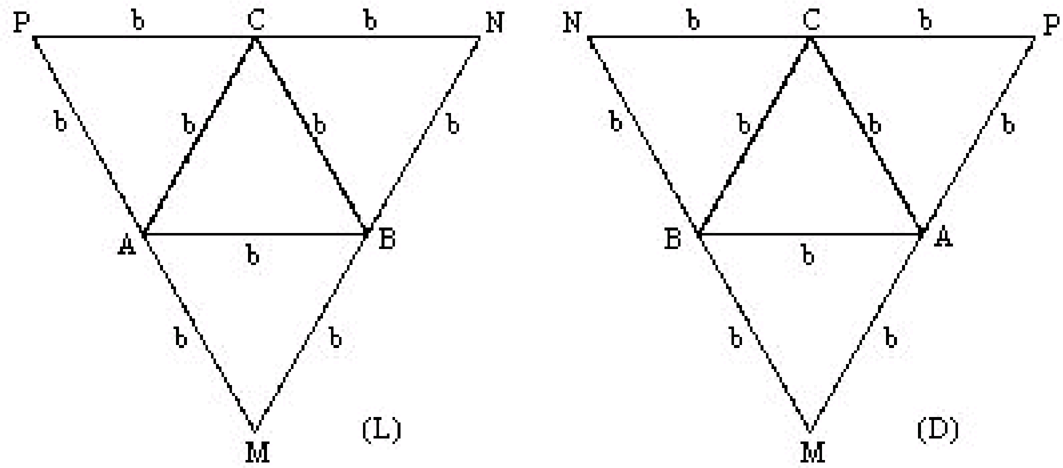

Figure 2: To construct regular tetrahedra by folding the paper on the sides of the central equilateral triangle.

Let us now consider the central equilateral triangle, and fold the paper on its sides. After turning the external equilateral triangles about these sides, their third vertices join together at the same point and we obtain regular tetrahedra. These are mirror images but they are not chiral since they are superposable. We can use the same method, if we require to build non-regular tetrahedra. Consider the two plane figures below, where $b + c > a > b > c$. It follows that the angles should satisfy $\widehat{MBN} = \widehat{PCN} = \pi - \widehat{PAM}$.

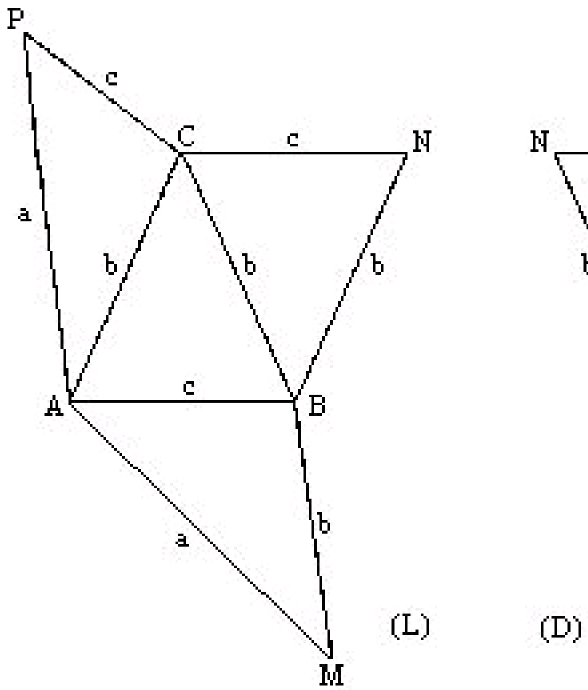

Figure 3: By folding the paper like in the foregoing figures, two non regular tetrahedra are obtained.

Analogously to figure (2), we can fold the paper on the sides of the central isosceles triangles and after turning the other triangles about these sides, we obtain two non-regular tetrahedra. These, in spite of being still mirror images are not superposable anymore. We say that they are enantiomorphous.

Let us try to understand this problem by posing another problem. We now restrict ourselves to think about in 2-dimensional structures. We invite the reader to follow the argument: we can cover all the plane with "tiles" like those of figure (2). Can we do the same if the "tiles" are like those given in figure (3)? To answer this question, it will be essential to know that the external angles with sides b and c as well as the internal angle with sides a are all of equal measure as can be seen straightforwardly. The answer to the posed question is in the negative. There are two fundamental ways in which we can try the covering process. The first is realized by using only (L) tiles or only (D) tiles. The other process is to use the (L) and (D) tiles alternatively. This second covering process succeeds into covering a strip in the plane. This strip be infinite if we use an infinite number of tiles. The former process does not lead to the covering of an infinite region even for an infinite number of tiles. We stress this point now in order to explain further the former process. Let us assume that the junction of tiles is at sides, a, b, like the figure (4), below. This junction model is enough for all the subsequent calculations. We can also make the junction of sides a, c, but this does not modify our conclusions.

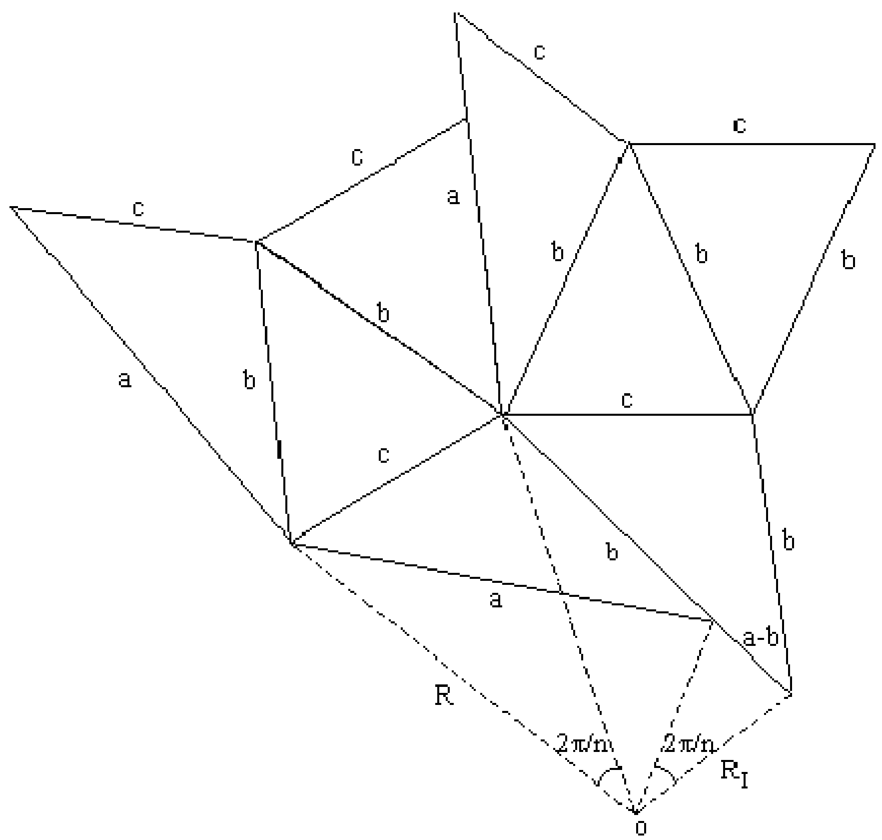

Figure 4: The junction of two (L) tiles.

2 The Tiling Process

Let us go back now to the generic problem of covering a surface with tiles. If this surface is the Euclidean plane, we know that we can cover it with equilateral triangles, squares, hexagons or other geometrical tiles in a periodic way. We can also cover it in a non-periodic way by using v.g. Penrose tiles. However, among the classes of tiles which cannot cover the plane, there are some which are able to cover a strip in the plane or to cover an annular region leaving a central region uncovered and limited by a regular polygon. An example of this are the tiles shown at figure (3). Let us suppose that from the geometrical construction above, figure (4), which correspond to the junction of the tiles we have chosen, we get these regular polygons of identical number of sides (n) but sidelengths c_p and $a_p - b_p$. A straightforward derivation by using elementary definitions and the sine law leads to

$$a_p - b_p = 2R_I\sqrt{1-t^2} \tag{1}$$

$$c_p = 2R\sqrt{1-t^2} \tag{2}$$

$$\frac{b_p}{(4t^2-1)\sqrt{1-t^2}} = \frac{R}{t} = \frac{R_I}{8t^4-8t^2+1} \tag{3}$$

where $t = \cos(\frac{\pi}{n})$ is given by the positive root of the equation

$$4t^2 - 2\frac{b_p}{c_p}t - 1 = 0 \tag{4}$$

From equations (1) to (3), we see that $\frac{2\pi}{n}$ is the angle subtended by the sides c_p and $a_p - b_p$ of the regular polygons.

This also leads to a restriction, since $t \leq 1$ and we have

$$2b_p \leq 3c_p \tag{5}$$

Our expressions for the functions $n(b_p, c_p), t(b_p, c_p), a_p(b_p, c_p), R(b_p, c_p)$ and $R_I(b_p, c_p)$ which give the solution of this plane geometry problem are given here for completeness. We have,

$$n(b_p, c_p) = \frac{\pi}{\arccos(t)} \tag{6}$$

$$t(b_p, c_p) = \frac{1}{4}(\frac{b_p}{c_p} + \sqrt{\frac{b_p^2}{c_p^2} + 4}) \tag{7}$$

$$a_p(b_p = 2tc_p(\frac{b_p^2}{c_p^2} - 1) \tag{8}$$

$$R(b_p, c_p) = \frac{c_p}{2\sqrt{1-t^2}} \tag{9}$$

$$R_I(b_p, c_p) = \frac{b_p(8t^4 - 8t^2 + 1)}{(4t^2 - 1)\sqrt{1-t^2}} \tag{10}$$

An analysis of these formulae will show that this tiling process is disconnected from that which uses only equilateral triangles. The necessary condition $b_p = c_p$ leads to $a_p = 0$.

We can now form a chain of non-regular tetrahedra by cutting all the sides of figures above and by folding the figure over the sides of the central isosceles triangles. The vertices of the angles with sides a_p units of length are left fixed in this process. The 3-dimensional chain is formed if we bound together the faces of the isosceles triangles referred above. Do the vertices of this structure correspond to those obtained by assuming points evenly spaced along a right circular helix?

The coordinates of evenly spaced points in a right circular helix of pitch $2\pi\alpha$ and unit radius, can be given by

$$x_j = \cos(j\omega); \qquad y_j = \sin(j\omega); \qquad z_j = \alpha j\omega \tag{11}$$

with $0 \leq j \leq p-1$.

These are the vertices of a 3-dimensional structure made of tetrahedra bounded together at common faces – the 3-sausage topology of ref.[2]. The lenght of their edges is given by the euclidean distances R_{ij} among vertices i,j, or

$$R^2_{j,j-1} = R^2_{j+1,j} = R^2_{j+2,j+1} = c^2_H = 16\beta(1-\beta) + 4\alpha^2\omega^2 \tag{12}$$

$$R^2_{j+1,j-1} = R^2_{j+2,j} = b^2_H = 4\beta + \alpha^2\omega^2 \tag{13}$$

$$R^2_{j+2,j-1} = a^2_H = 36\beta - 96\beta^2 + 64\beta^3 + 9\alpha^2\omega^2 \tag{14}$$

where $\beta = \sin^2(\frac{\omega}{2})$.

From the last equations, we can also write

$$a^2_H + 15b^2_H - 6c^2_H = 64\beta^3 \tag{15}$$

$$4b^2_H - c^2_H = 16\beta^2 \tag{16}$$

If tetrahedra are assumed to be regular, or, $a_H = b_H = c_H$, we get

$$\omega_R = 2.30058398302186298268611835145307213 7494 \tag{17}$$

$$\alpha_R = 0.26454000216541143401790656391011876 07981 \tag{18}$$

where the index R, stands for "regular".

A fundamental characterization of this structure is given by the Steiner Ratio concept [2]. It is defined to be the greatest lower bound or infimum among all 3-dimensional sets of R^3 of the ratio of the length of Steiner minimal tree and the length of minimal spanning tree.

In a foregoing work [1], we have derived an analytic formula for the Steiner Ratio as a function of ω, α. We have

$$\rho(\omega, \alpha) = \frac{1 + \alpha\omega \frac{\sqrt{1-2\cos(\omega)}}{\sqrt{2(1-\cos(\omega))}}}{\sqrt{\alpha^2\omega^2 + 2(1-\cos(\omega))}} \tag{19}$$

The value given in the literature [2] as the best upper bound for the Euclidean Steiner Ratio in R^3 coincides (in a 38 digit approximation) with that obtained in our calculation, or

$$\rho(\omega_R, \alpha_R) = 0.78419037337712224711083954778156877526539$$

An investigation in the plane $\alpha = \alpha_R$ can be made by solving a simple constrained optimization problem [1], and we get

$$\omega_I = 2.627864399093358959001772344582377864255 \tag{20}$$

We then have a new upperbound [1]

$$\rho(\omega_I, \alpha_R) = 0.7760017454914150111249155295940678190790 \tag{21}$$

3 The First Possibility. Direct Transcription from E^2 to E^3

We now study the possibility that the process which is adopted by Nature in the creation of 3-dimensional geometries is the same as that used in building the usually man-made 3-dimensional structures or

$$c_p = c_H; \qquad b_p = b_H; \qquad a_p = a_H \tag{22}$$

From equations (8) and (14)-(16), we can write

$$t^2(16\beta^2 - 3b_H^2)^2 = 2(b_H^2 - 4\beta^2)(9b_H^2 - 96\beta^2 + 64\beta^3) \tag{23}$$

The restriction (5) can be written here as

$$2b_H^2 \geq 9\beta^2 \tag{24}$$

In order to simplify the formulae, we write $b_H^2 = \chi$.

From equation (18), together with $0 < t^2 < 1$, we can formulate the problem of finding a feasible set F of values (β, χ), such that

$$F = F_1 \cap F_2 \tag{25}$$

$$F_1 = \{(\beta, \chi) | \chi - \chi_1 < 0, \chi - \chi_3 > 0, \chi - \chi_4 > 0\} \tag{26}$$

$$F_2 = \{(\beta, \chi) | \chi - \chi_2 > 0, \chi - \chi_3 > 0, \chi - \chi_4 > 0\} \tag{27}$$

and

$$\chi_1 = \frac{\beta^2}{9}(84 - 64\beta + 4\sqrt{153 - 38\beta + 256\beta^2}) \tag{28}$$

$$\chi_2 = \frac{\beta^2}{9}(84 - 64\beta - 4\sqrt{153 - 38\beta + 256\beta^2}) \tag{29}$$

$$\chi_3 = \frac{32}{3}\beta^2 \tag{30}$$

$$\chi_4 = \frac{9}{2}\beta^2 \tag{31}$$

The solution is

$$F = \{(\beta, \chi) | 0 < \beta < 0.3, \chi_3 \leq \chi \leq \chi_1\} \tag{32}$$

This leads, through equation $\beta = \sin^2(\frac{\omega}{2})$, to an interesting restriction for the ω-values

$$0 < \omega \leq 1.159279481 \tag{33}$$

This range is outside the range which we have adopted in our calculations of the foregoing contributions. We had therein [1],

$$\arccos(\frac{1}{3}) < \omega < 2\pi - \arccos(\frac{1}{3})$$

as we can see from definition of the set

$$V = \{(\omega, \alpha) | (\omega, \alpha) \in R_{++}, \arccos(\frac{1}{3}) \leq \omega \leq 2\pi - \arccos(\frac{1}{3}), \alpha \geq 0\} \quad (34)$$

4 A Possible Alternative. The Freedom of Nature in the Choice of a Convenient Geometry

If the construction of regular polygons is a real paradigm for transferring the geometrical expertise of 2-dimensional Euclidean geometry to 3-dimensional space, then all the 3-dimensional structures which we have considered in other sections, including the now famous 3-sausage [2] , cannot result from that 2-dimensional expertise. The point is that Nature would not be fool enough at trying to construct some regular polygons for which we now that there are not exact geometrical constructions. In spite of her infinite resources for increasing accuracy, the non-existence of a geometrical construction precludes this “natural” trial and error process. We see two ways of getting rid of this difficulty. The first is to consider the natural constructions in 3-dimensional space by their own, with no consideration for distances defined in a 2-dimensional setting. In this sense, Nature, contrary to human beings does not need the knowledge of 2-dimensional geometry to do geometry in 3-dimensional space. The existence of all the structures which we have been studying in the modelling of macromolecules standing as examples of this fact. The second possibility is the consideration that Nature can follows different rules in her building of 3-dimensional structures as biomacromolecules. In order to give an example, let us assume that the “transcription” of the geometrical knowledge from 2-dimensional space to build a structure in 3-dimensional space is made, instead of that given into equations (16), by the alternative,

$$c_p = kc_H^2; \quad b_p = kb_H^2; \quad a_p = ka_H^2 \quad (35)$$

where k is a dimensional constant.

We should firstly observe that $t = \cos(\frac{\pi}{n})$ is independent of k, according to equation (7).

From equations (8), (14), (15) and (22), we can write,

$$t(-15b_H^4 + 128\beta^2 b_H^2 - 256\beta^4) = 2(b_H^2 - 4\beta^2)(9b_H^2 - 96\beta^2 + 64\beta^3) \qquad (36)$$

The restriction (5) is now

$$5b_H^2 \geq 24\beta^2 \qquad (37)$$

As in the last derivation, we make $b_H^2 = \chi$.

Analogously, from equation (31), by making use of $0 < t = \cos(\frac{\pi}{n}) < 1$, the problem is then reduced to find the feasible set G of values (β, χ) such that

$$G = G_1 \cap G_2 \qquad (38)$$

where G_1, G_2 are given by

$$G_1 = \{(\beta, \chi) | \chi - \chi_1 < 0, \chi - \chi_3 < 0, \chi - \chi_4 > 0\} \qquad (39)$$

$$G_2 = \{(\beta, \chi) | \chi - \chi_2 > 0, \chi - \chi_3 < 0, \chi - \chi_4 > 0\} \qquad (40)$$

and

$$\chi_1 = \frac{\beta^2}{33}(196 - 64\beta + 4\sqrt{289 - 521\beta + 256\beta^2}) \qquad (41)$$

$$\chi_2 = \frac{\beta^2}{33}(196 - 64\beta - 4\sqrt{289 - 521\beta + 256\beta^2}) \qquad (42)$$

$$\chi_3 = \frac{32}{3}\beta^2 \qquad (43)$$

$$\chi_4 = \frac{24}{5}\beta^2 \tag{44}$$

The solution can be written as:

$$G = \{(\beta, \chi)|0 < \beta < 0.95, \chi_4 \leq \chi \leq \chi_1\} \tag{45}$$

This result then leads now to the new restriction for the ω-values

$$0 < \omega \leq 2.690565842 \tag{46}$$

This is really interesting. The new range includes the values and which were the object of exhaustive research in ref. [1] . It remains to be seen, if another interpretation of the Euclidean distances in the plane, in their adoption to create structures in 3-dimensional space, can extend the right end to reach the value $2\pi - \arccos(\frac{1}{3})$ which helps to define the V-set into equation (28).

5 An Interesting Result. The Discard of Euclidean Distance

As an example of the powerfulness of this proposal (equation (19)), we give the results of an application with the values ω_I and α_R as derived in section (2) in a 40 digits approximation, or

$$\omega_I = 2.627864399093358959001772344582377864255$$

$$\alpha_R = 0.2645400021654114340179065639101187607981$$

we then get

$$\beta = 0.9354591986653898241824062787969181878491 \tag{47}$$

and from equations (11)-(13),

$$c_H^2 = 2.899079114894460082043518152354820039815 \tag{48}$$

$$b_H^2 = 4.2251054281943880885781322767789151110\,63 \quad (49)$$

$$a_H^2 = 6.4086321738721587007884566386662233337\,76 \quad (50)$$

From equation (7), we have

$$t = 0.98301696023708132397043028689663817106\,53 \quad (51)$$

and from equation (6),

$$n = 17.022000628977696186142552895720305617871 \quad (52)$$

This should be considered as a good result. The meaning is that we can have a better 3-dimensional structure, by starting from the construction of a regular 17-side polygon. It is worth to strive for improving the accuracy, since a polygon like that is the first non-trivial case of exact geometrical construction, according to a famous result of Gauss.

In summary, we consider the values of b_H and c_H obtained from equations (12) and (11). If the sides b_p and c_p of the of the triangle to be constructed, are given by

$$b_p = kb_H^q; \qquad c_p = kc_H^q \quad (53)$$

where q is a rational number and k a dimensional constant, we then get from equations (7) and (8),

$$t_q = \frac{1}{4}(y^q + \sqrt{y^{2q} + 4}) \quad (54)$$

and

$$a_p = 2kc_H^q t_q(y^{2q} - 1) \quad (55)$$

where $y = \frac{b_H}{c_H}$.

We now ask what is the pair of values (ω, α) and the q-value such that we also have,

$$a_p = ka_H^2 \quad (56)$$

where a_H is given by equation (13), or

$$a_p = 2^{\frac{-1}{q}} c_H (y^q + \sqrt{y^{2q}+4})^{\frac{1}{q}} (y^{2q}-1)^{\frac{1}{q}} \tag{57}$$

We also note that the asymptotic value of the last formula is

$$a_{H_{ASYMP}} = \frac{b_H^3}{c_H^2} \tag{58}$$

Equation (51) is only satisfied by $q = 2$, when $\omega = \omega_I$ and $\alpha = \alpha_R$, as we could expect from the analysis done above in this section. The value $q = 1$, corresponding to configuration (16) is discarded as can be seen from restriction (27) and figure (5) below

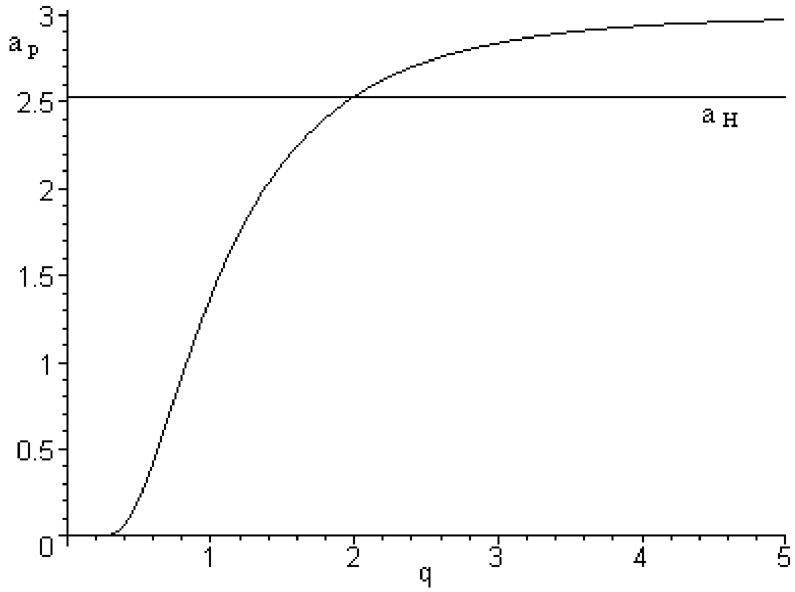

Figure 5: The $q = 2$ value satisfies equation (50) and the $q = 1$ value is discarded for $\omega = \omega_I$ and $\alpha = \alpha_R$.

The structure of the problem treated above restricts our speculations to $\frac{3}{2}c_H > b_H > c_H$. The configuration corresponding to the pair (ω_R, α_R) which has $b_H = c_H$ is disconnected from the values considered in the last study. This is in the sense that it cannot be reached by a continuous deformation by starting from b_H, c_H values within the allowed range. To reach that configuration it would be like to have a first order phase transition with abrupt transformation. It will be also worthwhile to study the behaviour of the function

$$n_q = \frac{\pi}{\arccos(t_q)} \tag{59}$$

near the value $y = 1$ $(b_H = c_H)$. We have,

$$n_q \approx 5 + \frac{5q(5+\sqrt{5})}{\pi\sqrt{10-2\sqrt{5}}}(y-1) \tag{60}$$

All plane configurations with $b_H > c_H$, start from a regular pentagon and they end in a configuration with a maximum q-value. This can be seen from the analysis of the function (53) together with equation (48). For the starting point

$$\lim_{q \to 0} n_q = 5 \tag{61}$$

For the maximum q-value, we have, correspondingly,

$$t_q = 1$$

or

$$q_{max} = \frac{0.4054654084}{\ln(y)} \tag{62}$$

It looks remarkable to have the regular heptadecagon as the plane configuration with the greater number of sides, if we adopt the values (ω_I, α_R) for calculating n_q, equation (53). For these values, we got from equation (56),

$$q_{max} = 2.153001207 \tag{63}$$

The exact q-value for the heptadecagon being

$$q = 1.999597686 \tag{64}$$

These values are to be compared with the value $q = 2$, which was used for obtaining the value reported into equation (46). In table 1, by working with the value (ω_I, α_R), we can observe the behaviour of the function n_q for some characteristic q-values. These correspond to different realizations in 3-dimensions of the measures of angles and lengths usually studied in 2-dimensional Euclidean geometry. The "natural" interpretation ($q = 1$) should be discarded here, as we have emphasized in figure (5) above, since it leads to a n_q value which we cannot approximate by an integer. Moreover, when we try to join the tiles (L) and (D) from figure (3), the best we can do is to construct an almost regular heptagon and we know that is not possible to improve our construction without limit on accuracy, by the hindrance of a theorem which precludes exact geometrical construction. This will be not a big problem if we choose instead, the value $q = 2$ and we improve our measurements without any hindrance, since we are approaching the construction of the heptadecagon.

The behaviour of the n_q function

q	$\mathbf{n_q}$
0	5
1/4	5.255033098
1/3	5.352548649
1/2	5.371026676
1	6.510946233
2	17.02200052

Table 1: The n_q values from chosen q-values corresponding to different realization of 3-dimensional geometry with a common 2-dimensional euclidean origin. All the calculations were done with the values (ω_I, α_R).

We now go back to the approximation (54) and we note that the configuration with $b_H = c_H$ or (ω_R, α_R) is disconnected from all those which we have been studying here, as we have emphasized already. This configuration corresponds to the central picture in figure (6). It is a piece made of twenty tetrahedra (unit cells) of the 3-sausage of ref. [2]. In the left side of the same picture, we see a configuration built with levogirous tiles and correspondingly, levogirous tetrahedra. In the right side is the configuration for dextrogirous tiles and dextrogirous tetrahedra. We have chosen to use equal number of tetrahedra for all of them and they were built on scale. It is interesting to note that the two configurations built from non-regular tetrahedra have increased their size as compared with this piece of the 3-sausage. In this last one, we can see three right handed helices. In the left side configuration, we have two right handed helices and two left handed helices on the right side configuration (we look at the sequence of the smallest edges). The upsurge of geometrical chirality, it is a process for which we have to find a dynamical description. It is at this point, outside of the scope of this publication. However, we notice here, for the first time that the Steiner Ratio of the two lateral configurations in figure (6) is 1% lesser than that for the central configuration. The remarks and observations made here should be useful in the discovery of that sort of perturbation which is able to drive the central configuration to one of the two others. To drive it to the emergence of life, with a divine bias for one of them.

Figure 6: The picture in right hand side corresponds to a configuration with two left handed helices. The central picture and the left hand side one have three and two right handed helices on their structures, respectively.

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