The Kinematics of a Framework Presented by H. HARBORTH and M. MÖLLER

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Abstract.

We consider a model of interlinked tetrahedra which was described by H. HARBORTH and M. MÖLLER in [1]. It consists of 16 congruent regular tetrahedra connected via 32 spherical joints (in the vertices of the tetrahedra). In this arrangement they define a *saturated packing*. There every vertex of a tetrahedron is exactly linked to one of another tetrahedron. Although the Grübler formula gives a theoretical degree of freedom $f = -6$ for this kinematic chain, and therefore the model should be rigid, we demonstrate that this mechanism admits at least a two-parametric self- motion in the general position. Further we consider a special, degenerate case of this model, which again admits a two-parametric self-motion. This motion contains geometrically interesting positions regarding the cross-section of possible prismatic channels through the model. These channels occur as empty space through the model as the tetrahedra are considered to be solids. We present positions with vanishing channels and with a cross section of area a^2 for tetrahedra with edge length a.

1. Introduction.

A set of congruent regular triangles in the plane (congruent regular tetrahedra in the space) is called a *saturated packing*, if every vertex is connected to exactly one vertex of a triangle (tetrahedron) of the set. In addition we don't want the triangles (tetrahedra) to interfere with each other. In the Euclidean plane there exists an example involving $n = 42$ regular triangles [1]. But it is still unknown if there exist examples for $n \leq 42$.

We can easily see, that this 2D-example can be extended to a saturated packing of 84 regular tetrahedra in space. A more general procedure of this

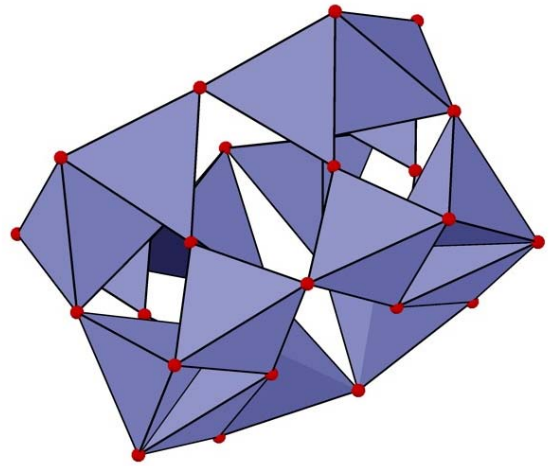

Figure 1: Saturated Packing of 16 tetrahedra

type (with layer construction) can be used for infinite cases and is presented in [4].

Saturated packings of regular tetrahedra are geometric models of molecules called 'Zeolites': Zeolites consist of tetrahedra-shaped SiO_4 or AlO_4 structures which are linked with one common Oxygen-atom and form cristalline structures with pores (for more details see [3], 456-459). As Zeolites can adsorb molecules smaller than their pores, they can be used as molecular sieves.

The 'smallest' saturated packing in 3-space which is presently known, consists of 16 tetrahedra and was first presented by H. Harborth and M. Möller in [1] (see figure 5). It consists of 16 rigid bodies (the congruent regular tetrahedra) which are interlinked via 32 spherical joints. The theoretical degree of freedom for this mechanism takes on the value $f = -6$.

We will consider this model and some of its kinematic properties in chapter 2. A physical model can be generated as framework of 96 rods. It seems to admit some infinitesimal or finite self-motion. The aim of chapter 2 is to perform a kinematic study of this interesting kinematic chain which has some similarity with the Grünbaum framework of 10 regular tetrahedra. But there the tetrahedra are intersecting. The kinematics of this famous framework was worked out by H. STACHEL in [5].

Chapter 3 is devoted to the kinematic study of some 'degenerate case' and the 'chanels' of this model.

2. Two parametric motion.

Since the model remains symmetric with respect to two mirror planes (see figure 3), it is sufficient to study one fourth of it. The linking vertices in the mirror planes will stay together anyway. This fourth of the model is built up by a chain of 4 regular tetrahedra (labeled $1, 2, 3, 4$ in the figures 3 and 4), which are interlinked via spherical joints centered in the points O, A, B, C, D. The 6 remaining vertices E, F, G, H, I, J of the four tetrahedra are 'unsaturated' for the moment - later they will be used to interlink with neighboring chains. The points O, A, B, C, D form 4 regular triangles meeting in the point O. Two of them (ABO and CDO) belong to tetrahedra of the packing, two remain 'empty'. These 4 regular triangles form the boundary of 'half an octahedron' (i.e. a part of a pyramid with common vertex O).

The free edges AD and BC of the empty triangles are edges of the tetrahedra labelled 3 and 4 in figure 6.

This chain admits the following self-motions:

- A one-parametric deformation of the half-octahedron (where the distances of the vertices B, D and A, C vary).
- Two independent rotations of tetrahedron 3 and tetrahedron 4 about their edges AD and BC, resp.

Now we will study the self-motions of this partial chain of the mechanism. One basic figure in this chain is the half - octahedron O, A, B, C, D which in any position has two planes of symmetry. They will be used as coordinate planes of a Cartesian frame with origin in O (see Figure 2). The self-motion of this half-octahedron can be parametrized by angles α and β

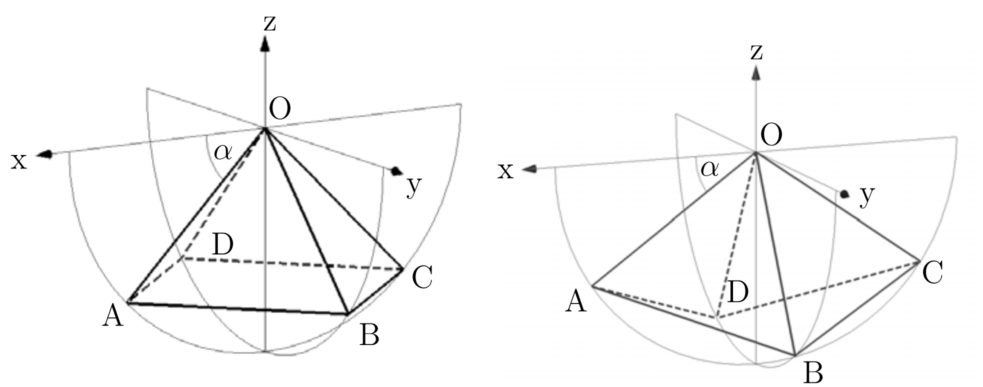

Figure 2: Half an octahedron

$$A(\alpha) = \begin{pmatrix} \cos\alpha \\ 0 \\ -\sin\alpha \end{pmatrix} \qquad B(\beta) = \begin{pmatrix} 0 \\ \cos\beta \\ -\sin\beta \end{pmatrix} \tag{1}$$

$$C(\alpha) = \begin{pmatrix} -\cos\alpha \\ 0 \\ -\sin\alpha \end{pmatrix} \qquad D(\beta) = \begin{pmatrix} 0 \\ -\cos\beta \\ -\sin\beta \end{pmatrix} \tag{2}$$

with the additional condition for the edge-lengths (e.g. $\overline{AB} = 1$)

$$1 = 2\sin\alpha\ \sin\beta.$$

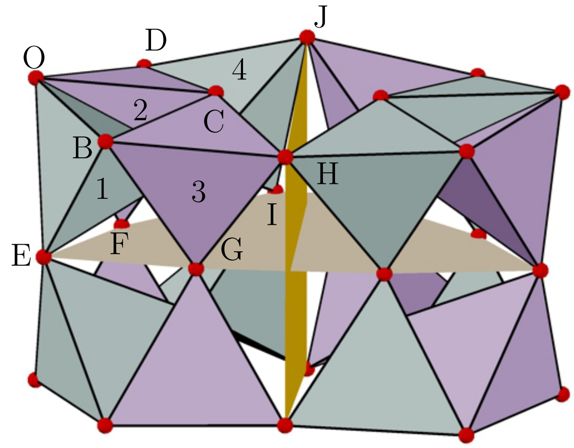

Figure 3: Model with its two planes of symmetry

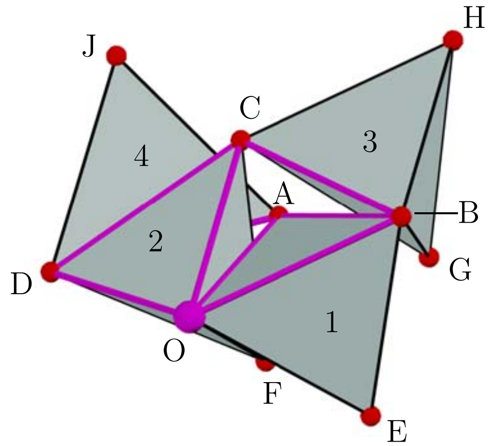

Figure 4: Half-octahedron in one fourth of the model: Vertex O and basic quadrangle $ABCD$

Therefore and for reasons of symmetry we can restrict the range of α and β to $[\pi/6, \pi/2]$. The partial chain of our 4 tetrahedra is completed by adding the two tetrahedra $1, 2$ and the two tetrahedra $3, 4$ (see Figure 4). The two free vertices of the tetrahedra 1 and 2 (labelled E and F in figure 4) then are given by

$$E = \frac{1}{3} \begin{pmatrix} \cos\alpha + 2\sqrt{2}\cos\beta\ \sin\alpha \\ \cos\beta + 2\sqrt{2}\cos\alpha\ \sin\beta \\ -\sin\alpha - \sin\beta + 2\sqrt{2}\cos\alpha\ \cos\beta \end{pmatrix} \tag{3}$$

$$F = \frac{1}{3} \begin{pmatrix} -\cos\alpha + 2\sqrt{2}\cos\beta\ \sin\alpha \\ -\cos\beta + 2\sqrt{2}\cos\alpha\ \sin\beta \\ -\sin\alpha - \sin\beta - 2\sqrt{2}\cos\alpha\ \cos\beta \end{pmatrix}. \tag{4}$$

Each of the two remaining tetrahedra $3, 4$ has two free vertices. We call them G, H for tetrahedron 3 and I, J for tetrahedron 4. Apart from the motion of the half-octahedron parametrized by the angle α, these vertices are movable along a circle around the midpoint of the connecting edge. For each α this leads to two circles k_1 for tetrahedron 3 and k_2 for tetrahedron 4. They can be parametrized by

$$k_1(s) = \frac{1-\cos s}{2}\begin{pmatrix} \cos\alpha \\ -\cos\beta \\ -\sin\alpha - \sin\beta \end{pmatrix} + \sin s \begin{pmatrix} \sin\alpha\ \cos\beta \\ -\cos\alpha\ \sin\beta \\ \cos\alpha\ \cos\beta \end{pmatrix} \tag{5}$$

$$k_2(t) = \frac{1-\cos t}{2}\begin{pmatrix} -\cos\alpha \\ \cos\beta \\ -\sin\alpha - \sin\beta \end{pmatrix} + \sin t \begin{pmatrix} -\sin\alpha\ \cos\beta \\ \cos\alpha\ \sin\beta \\ \cos\alpha\ \cos\beta \end{pmatrix} \tag{6}$$

with $s, t \in [0, 2\pi]$.

As we want to complete the model via mirror images of this part, we have the constraint that the vertices E, F, G and I have to lie in a plane. For every position of the half-octahedron (depending of the angle α) the points E and F are fixed. We can now choose a point on one of the circles e.g. $G := k_1(s)$ on k_1. We compute the position of $I := k_2(t)$ as the intersection of the circle k_2 and the plane containing E, F and G. This planarity condition can be interpreted as a relation between the parameters s and t on k_1 (5) and k_2 (6). This is guaranteed by the vanishing of the determinant of vectors connecting the corresponding points:

$$0 = Det(\vec{EF}, \vec{EG}, \vec{EI}) \tag{7}$$

This condition can be used to determine the variable t depending of s and α. It is a quadratic equation for $\tan(t/2)$ depending on the parameters α and s. Within some limits for α and s there exist real solutions for $t = t(s, \alpha)$. This way we have got a chain of 4 regular tetrahedra which at least admits a finite two-parametric motion which does not disturb the planarity condition. There the angles α and s can be interpreted as parameters. $t = t(s, \alpha)$ has to fulfill (7).

We reflect this part in the plane $[E, F, G, I]$ and gain a chain of 8 regular tetrahedra with 4 unsaturated vertices: The vertices H, J and their reflected images H^*, J^*. As the lines $[H, H^*]$ and $[J, J^*]$ are parallel the four points H, H^*, J, J^* are complanar. Reflection of our 8 tetrahedra in this plane will end up in a saturated chain of 16 regular tetrahedra. The finite two-parametric motion (independent parameters α and s) of one fourth of the mechanism induces a two-parametric self-motion of the whole structure.

We sum up in

Theorem 1: The original model of H. HARBORTH and M. MÖLLER of a saturated chain of 16 tetrahedra linked via 32 spherical joints admits at least a two-parametric self-motion. The two parameters are the angles α and s used in (1),(2), (3),(4) and (5),(6).

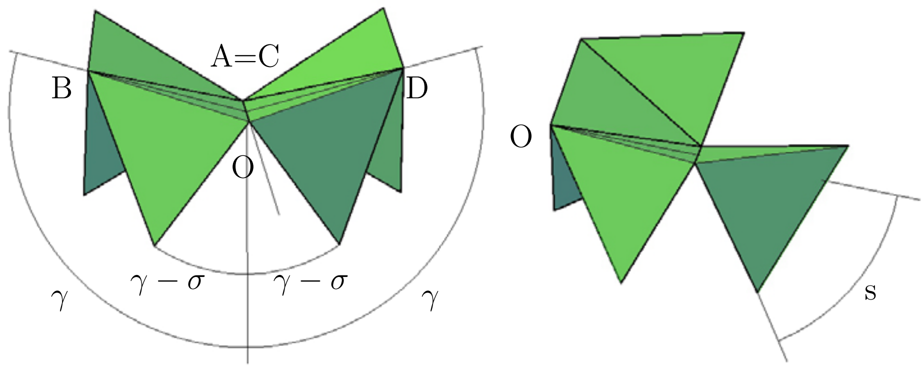

Figure 5: The two motion-parameters γ and s in the degenerate case

3. A Degenerate Case

We now consider the kinematic chain from above without the restriction of possible self-intersections of the interior of the tetrahedra.

The rigid bodies (the tetrahedra) are interpreted as solids. A 'weak restriction of saturation' shall allow vertices, edges or faces of different tetrahedra to coincide with the boundary of another tetrahedron. We still want to keep the topological structure of the connections of the vertices from the former model, but the vertices can also coincide with more vertices of other tetrahedra. Then the half octahedron may 'collapse' in the following sense: the points A and C coincide throughout the whole self-motion. This *degenerate case* will be discussed further on. It can be seen as the limit of a saturated packing. Here we have $\alpha = \pi/2$ for all possible self-motions.

But we achieve a second free parameter for the self-motions in this degenerate case too: The vertices B and D lie on a circle with the midpoint of $OA = OC$ as center. If the angle between two faces of the regular tetrahedron is named σ the angle between tetrahedra 1 and 2 is $2(\gamma - \sigma)$ (see figure 5). The whole system is symmetric with respect to a plane through the edge OA. The second parameter of movability is the same as in the general case - the angle s.

In this degenerate case we have got a highly symmetric model with three planes of symmetry (see figure 6) which again admits at least a two parametric self-motion.

Therefore our 'non-degenerate' mechanism has a bifurcation at $\alpha = \pi/2$. In this position it can run into the two-parametric self-motion of chapter 2 or into a further two-parametric self-motion (belonging to the degenerate case).

We sum up in

Theorem 2: The "degenerate model" admits at least a two-parametric self-motion. The two parameters are the angles γ and s.

A (prismatic) hole through the model which allows smaller objects to pass

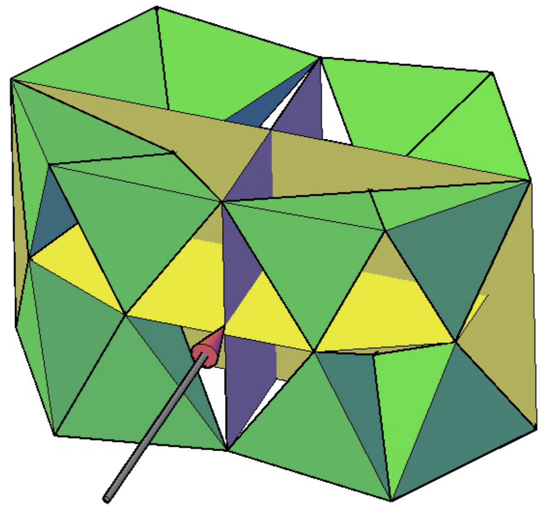

Figure 6: Degenerate case of the model with its three mirror planes

through and where no tetrahedra interfere with this flow, is called a (prismatic) channel. It is easy to see that the motion of the model contains positions with vanishing channels. The parameters for one of these positions are:

$$s = s_0 = 0^\circ \tag{8}$$

$$\gamma = \gamma_0 = 125.264^\circ. \tag{9}$$

Although there is no channel through the object, there still is some octahedron-shaped empty space in the model.

We now concentrate on the channel in the direction of one of the lines of intersection of two mirror planes (see the arrow in figure 6). For the maximum cross section of this prismatic channel we formulate the constraints that the four edges of the hole form a planar square. This gets us to the two possible pairs of parameters:

$$(s_1, \gamma_1) = (-109.471^\circ, 150.504^\circ) \tag{10}$$

$$(s_2, \gamma_2) = (-76.760^\circ, 113.859^\circ). \tag{11}$$

In the first case, some of the tetrahedra interfere with the prismatic channel (see Figure 7). The second pair of parameters gives a position where the cross section of the corresponding prismatic channel has area 1 (the edges of the tetrahedra have length 1).

We can state

Theorem 3: The channels of the packings in the degenerate case have cross sections with varying area $A(\gamma, s)$. According to (8), (9) and (11) there exist positions with vanishing and maximal area (e.g. $A(\gamma_0, s_0) = 0$ and $A(\gamma_2, s_2) = 1$).

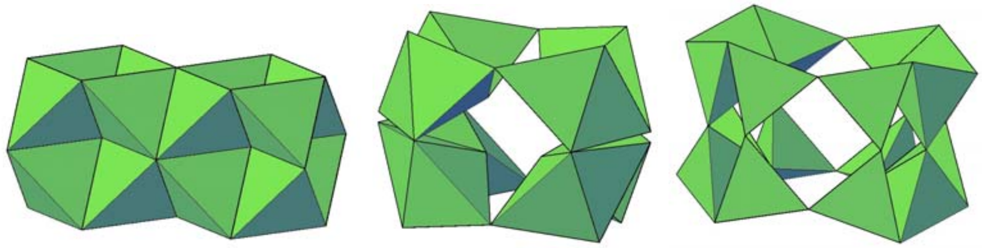

Figure 7: Positions of the model where the channel reaches the minimal and the maximal cross section

4. Conclusion

We performed a kinematic study of a saturated packing of 16 tetrahedra. Packings of this kind are used as models of zeolites. Some of their geometric properties do have chemical interpretations. The general saturated model (presented by H. HARBORTH and M. MÖLLER [1]) admits at least a two-parametric self-motion. In this paper it was parametrized by two independent angles α and s. At $\alpha = \pi/2$ there is a bifurcation. At this position the kinematic chain can split into a further two-parametric self-motion. It belongs to self-motions of an interesting 'degenerate case' of this kinematic chain. It can be seen as the limit case of the saturated packing from above. It is interesting to know prismatic channels through the model and the area of their cross sections. In the degenerate case we could determine the maximal and minimal value of these areas. Although the degenerate case has no direct chemical interpretation this result allows to estimate the behavior of the non-degenerate zeolite.

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