

## Several Attempts Concerning Quasicrystals from *Katachi* Interest

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The author is one of the organizers of the interdisciplinary cooperation based on *Katachi* as the key word, which is similar to that of *Symmetry*. He has investigated several problems relating with quasicrystals in this context since 1985.

Some attempts among them are briefly mentioned.

### 1. Before Quasicrystal

About 25 years ago, The author realized that his main interest is rather geometrical. His research subject till then was many-body or correlation problems in both of quantum and classical physics. He found common difficulty is brought by repulsive interaction as the volume exclusion effect. The effect is rather qualitative and it is not easy to quantify because it depends on how particles keep away each other in space. In classical problems as in high density simple liquids, the volume exclusion effect causes the remarkable decrease of entropy in disordered branch. In quantal system as in electron liquids in a narrow band, the strong repulsion causes the increase of kinetic energy by the localization of electron.

In order to estimate such effects, the property of the space is necessary to know. It was the motivation which drove me to geometrical problems. He explored a possibility of statistical or stochastic geometry together with his colleague Tanemura with the purpose to investigate the high density configuration [1]. We introduced the concept of geometrical neighbor and local order analysis based on Voronoi tessellation [2]. Another attempt was to study whether icosahedral structure is more stable from the viewpoint of electronic energy [3]. The author's view on the eve of the revolution of crystallography by the discovery of quasicrystal [4] was described in 1983 [5].

### 2. 3D Penrose Transformation

Thus, The author was rather familiar to icosahedral symmetry when he learned the discovery of the metallic phase with long ranged orientational order and no translational symmetry [4] by the information from A. L. Mackay. he had been believing that Penrose tiling [6] had been already extended to 3-D succeeded by Mackay [7]. The author tried to understand the structure. It was natural for him to choose two rhombohedral elements so long as 12 five-fold axes are taken. What he aimed was to construct the smallest similar structure of two sets of 8 vertices of these two elements. After some trial, he realized that it is impossible for inflation

rate  $\tau$  (the golden ratio) due to Mackay. The value is related with the following eigenequation of  $2 \times 2$  matrix:

$$\begin{pmatrix} 3 & 2 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau^3 \begin{pmatrix} \tau \\ 1 \end{pmatrix} \quad (1)$$

Reminisce that the corresponding equations for 1-D and 2-D are respectively

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau \begin{pmatrix} \tau \\ 1 \end{pmatrix} \quad \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau^2 \begin{pmatrix} \tau \\ 1 \end{pmatrix} \quad (2)$$

He guessed the following general relation for arbitrary  $D$  dimension

$$\begin{pmatrix} f_{D+1} & f_D \\ f_D & f_{D-1} \end{pmatrix} \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau^D \begin{pmatrix} \tau \\ 1 \end{pmatrix} \quad (3)$$

where  $f_n$  is the  $n$ th term of Fibonacci sequence. The corresponding inflation rate is always  $\tau$ . The author tried further and eventually found the solution in transformation method (T-model) at the end of May in 1985 [8]. His answer was multifold in the sense that there remains some degree of freedom undecided in the structure. The knowledge of the research of Higher dimensional cubes by Miyazaki was very helpful. He had already some intuition to the golden zonohedra, two 6-hedra, a 12-hedron, a 20-hedron, and a 30-hedron from the beginning of the trial. The inflation rate is  $\tau^3$  corresponding to the eigenequation

$$\begin{pmatrix} 55 & 34 \\ 34 & 21 \end{pmatrix} \begin{pmatrix} \tau \\ 1 \end{pmatrix} = \tau^9 \begin{pmatrix} \tau \\ 1 \end{pmatrix} \quad (4)$$

The value  $\tau^3$  is the ratio of the main diagonal of two rhombohedra. In other words, they respectively correspond to the two cases of the first return to the three-fold axes. He regarded it as lucky that the answer lies in the possible minimum value of the inflation rate.

### 3. T-model vs. P-model; Symmetry vs. Homogeneity

The author noted that the coordinates of the vertices are expressed as a set of 6 integers and then they can be regarded as the projection of 6-D simple lattice in some sense. But, he could not find the principle of the projection. Most people used the projection model (P-model) because it is useful. One can calculate physical properties by computer basing on the P-model even without knowing anything about the feature of the structure. It took nearly a year for the author to see the relation between T-model and P-model. Finally he realized that the feature of the P-model is homogeneity and the local symmetry is not so high. The freedom in T-model is useful to design various structures basing on the symmetry idea. For example, fractal hierarchy of symmetry [9].

### 4. Geometrical Long Range Order and Physical Long Range Order

Both of T-model and P-model are deterministic though they contain a kind of hidden parameter. Note that a physical long range order is stable against thermal fluctuation or disturbance even in finite temperatures. Even if we can understand the stability of periodic

order, the stability of quasicrystal is more difficult to understand. It is the one of the most basic problem in physics of quasicrystal.

## 5. Graphic Geodesic Line: Characterization of some Intermediate Range Order

A graphic geodesic line is defined for arbitrary triangular network [10]. It is a series of triangles two of whose three edges are respectively common with each neighboring triangles. For regular triangular lattice, all the geodesic lines have infinite length and belong to one of three sets of (*topologically*) parallel lines. They are locally straight but globally meander by local curvature. The 2-D Penrose tiling is triangulated by drawing the minor diagonals of rhombi. The analysis is completely performed since they are classified into finite number of categories. A similar analysis was carried out, But, the situation is furthermore complicated. It seems to have a kind of spatial chaos, in which the behavior of a geodesic line is not predictable. The conclusion, however, is still tentative.

## 6. Proportional Representation in Election System and Crystallography

The allocation of diet seats to parties in proportion to the votes is the problem to find the most suitable lattice point. It is closely connected with generalized crystallography. The relation between De Hondt scheme and Saint Lague scheme was shown from the point of view of crystallography [11].

## 7. Rod Composition and Penrose tiling

The author and his collaborators are trying to construct the crystallography of rod system [12] [13]. General relation of two rods are twisting and it is not so easy intuitively to see. There are no mirror symmetry with only some exception in the rod systems. It is useful as composite material [14]. Recently, Hizume succeeded to extend the rod construction of icosahedral symmetry as *Star Cage* [15], which was first carried out by 30 rods by Coffin [16]. It is based on 2-D Penrose tiling. What is impressive about it is that the 2-D Penrose tiling designed for 2-D quasiperiodic pattern is valid for 3-D rod construction.

## 8. Concluding Remarks

The author's attitude to research is basically to solve a kind of puzzles and to enjoy it. Physics should be more adventurous! Quasicrystal is just the problem of such a type, as the insight by Shechtman *et al.* and the prediction by Penrose had actually showed. A monograph on quasicrystals, in Japanese, is now in preparation from this point of view.

## References

- [1] T. Ogawa and M. Tanemura; *Progress of Theoretical Physics*, 51 (1974), 399.

- [2] M. Tanemura, Y. Hiwatari, H. Matsuda, T. Ogawa, N. Ogita, and A. Ueda; *Progress of Theoretical Physics*, 58 (1977) 1070.
- [3] T. Ogawa; *Zeitschrift für Physik*. B28 (1977), 73.  
T. Ogawa and S. Nara; *Zeitschrift für Physik*. B33 (1978), 69.
- [4] D. Shechtman, I. Blech, D. Gratias and J. W. Cahn; *Physical Review Letters*, 53 (1984), 1951.
- [5] T. Ogawa; in *Topological Disorder in Condensed Matter* Eds. F. Yonezawa and T. Ninomiya, (Springer, 1983), p. 60.
- [6] R. Penrose; *Journal of the Institute of Mathematics and Its Applications*. 12, (1974), 271.
- [7] A. L. Mackay; *Soviet Physics Crystallography*. 26 (1981), 517.  
A. L. Mackay; *Physica*, 114A (1982), 609.
- [8] T. Ogawa; *Journal of Physical Society of Japan*, 54 (1985), 3205.  
T. Ogawa; in *Science on Form* Eds. Y. Kato et al. (KTK Sci. Pub., Tokyo / Reidel, 1986) p. 479.  
T. Ogawa; in *Morphology and Growth Unit of Crystals* Ed. I. Sunagawa (Terra Pub. Co., Tokyo, 1989) p. 53.
- [9] T. Ogawa; *Materials Science Forum*, 22-24. (1987), 187.
- [10] T. Ogawa and R. Collins; in *Quasicrystals* Eds. T. Fujiwara and T. Ogawa (Springer, 1989) p. 14.
- [11] T. Ogawa and T. Ogawa; in *Quasicrystals* Eds. K. H. Kuo and T. Ninomiya (World Scientific, 1989) p. 394.
- [12] Y. Teshima, Y. Watanabe and T. Ogawa; in *KATACHI  $\cup$  SYMMETRY* (Springer, 1996), p. 239.  
Y. Teshima, Y. Watanabe and T. Ogawa; *JRDC Forum for Multi-Disciplinary Researches*. (1995).
- [13] M. O'Keeffe; *Acta Crystallography*. 33 (1977) 914.  
M. O'Keeffe; *Acta Crystallography*. A48 (1992), 879.
- [14] A. Hijikata and K. Fukuda; *Journal of Japanese Society of Composite Materials*, 18 (1992, in Japanese), 231-238.  
K. Fukuda; *Journal of Japanese Society of Composite Materials*, 21 (1992, in Japanese), 51-60.
- [15] A. Hizume; *Forma*, 9, (1994), 259.  
A. Hizume; *KATACHI  $\cup$  SYMMETRY Extended Abstract* (1994) p. 99.
- [16] S. T. Coffin; in *The Puzzling World of Polyhedral Dissection*, (Oxford University Press, 1990).