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Symmetry of life in crystals

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The results of the study of quasicrystals matrix models are presented, which confirm the hypothesis that each quasicrystal has corresponding quasiorthogonal matrix associated with it, the golden ratio matrix meets the D.Shechtman quasicrystal. It is concluded that for the ordered structures consisting of two endlessly recurring units, a modular two-level golden ratio matrix may be a model reflecting the structure elements. The main interest here is in the indication of the prospects: both the materials and the matrices can have different structures, and the matrices can be involved in predicting the existence and then in analyzing the materials.
Keywords: quasicrystal, quasiorthogonal matrix, golden ratio matrix.

В статье приведены результаты исследования матричных моделей квазикристаллов, подтверждающие гипотезу, что каждому квазикристаллу отвечает асоциированная с ним квазиортогональная матрица, квазикристаллу Д.Шехтмана отвечает матрица золотого сечения. Сделан вывод, что для упорядоченных структур, состоящих из двух бесконечно повторяющихся фрагментов, моделью, отражающей детали строения, может являться модульно двухуровневая матрица золотого сечения. Основной интерес состоит здесь в указании перспектив: ведь и материалы, и матрицы в состоянии иметь еще и другие виды, причем матрицы могут привлекаться для предсказания существования и затем для анализа материалов.

Симетрія життя в кристаллах. *М.О.Балонін, В.С.Суздаль.*
У статті наведені результати дослідження матричних моделей квазікристалів, які підтверджують гіпотезу, що кожному з квазікристалів відповідає асоційована з ним квазіортогональна матриця, квазікристалу Д.Шехтмана відповідає матриця золотого перерізу. Зроблено висновок, що для упорядкованих структур, які складаються з двох нескінченно повторюваних фрагментів, моделлю, що відображає деталі будови, може бути модульно-дворівнева матриця золотого перерізу. Основний інтерес полягає у вказівці перспектив: оскільки і матеріали, і матриці в змозі мати ще й інші види, причому матриці можуть залучатися для передбачення існування і аналізу нових матеріалів.

Introduction

According to the traditional view, the structure of a solid substance in the crystalline state is characterized by two major features: orderliness and periodicity. Thus, the crystal, according to the definition, is an ordered structure consisting (in theory) of an endlessly recurring unit (lattice cell). Ranging of the information in respect of the allowed crystals symmetry discriminated the crystalline lattice — an auxiliary geometric image introduced to analyze the crystal structure and the rotation axes of the second, third, fourth and sixth orders. These dogmas became so perpetuated in the official crystallography that opposing them led D.Shechtman who discovered the pentagrams in the experiments on ultra-fast cooling of aluminum and manganese alloys [1] to the Nobel Prize in 2011. The recognition of the finding was favored by the experiments of the British mathematician R.Penrose with two diamonds — the Penrose tiles built on proportions of the golden ratio forming repeating patterns with the long-range symmetry [2]. Such objects are now recognized and called quasicrystals.

In 1982, at the National Institute of Standards and Technology (USA) D.Shechtman studied the structure of aluminum and manganese alloy using electron diffraction. The picture seen by D. Shechtman is astonishing: ten bright points located around the central point. But this is just a part of the three-dimensional picture. After some time, having taken the pictures of the sample at different angles and adding a standard mathematical processing, he was able to determine how the atoms in the crystal are arranged. It turned out that they were located at the apexes of the icosahedron — a polyhedron assembled of 20 regular triangles. It is known that it is impossible to fill the space with icosahedrons so that they joint each other tightly, there are surely interstices which is impossible in crystalline objects. However, in 1984, D.Shechtman, I.Blech, D.Gratias and J.Cahn confirmed the symmetry of the fifth order on the electron-diffraction pattern of ultra-fast cooled aluminum and manganese alloy ($Al_{86}Mn_{14}$) [1]. The quasicrystals discovered by Shechtman are ordered but not periodic, i.e. they have no translational symmetry.

The space filling in the quasicrystals is very fancy; in fact there are two or three lattice cells, two or three types of lattice cells which are oddly combined without producing translational periodicity. Nevertheless, the structure possesses the long-range order. Diffraction pattern, i.e. the hosing of X-ray by the quasicrystal structure, is consist of clear sharp strictly located spots. In the same way as is in the crystal.

The symmetries of the fifth, seventh, and other orders prohibited in crystallography are the most common in nature. The rotational symmetry of the fifth order (72° angle) is the most effectively represented in plant life and in the simplest living organisms, particularly in some species of viruses and organisms of some sea dwellers (sea stars, sea urchins, colonies of green algae, radiolarians, and others). Flowers of many plants possess the rotational symmetry of the fifth order which until recently was not observed in inorganic nature. The quasicrystals show us the symmetry of life. We can say now that there is a transition link between the stone and the plant, which has a common symmetry.

At present there are hundreds of kinds of quasicrystals with icosahedral point symmetry, as well as with decagon, octagon and dodecagon one, but it was recognized that formation of such substances in nature is just impossible because the structure is extremely unstable. In 2009, scientists discovered the first natural quasicrystal in the rare mineral khatyrkite from Russian Far East. In the fragments of rocks collected in the Koryak Highland, natural quasicrystals reach the size of up to 200 μm. They consist of atoms of iron, copper and aluminum and have complicated structure with several (up to six) axes of the fifth order.

The following properties of the quasicrystals determine the possibility of their practical application: hardness, low friction coefficient, low thermal conductivity and unusual electricity-conducting properties. Today they are supposed to be used in a few fields, in particular, the development of quasicrystalline coatings and adding nanoparticles to alloys [3]. The most important field of application is the production of coatings. It is more promising than using the whole quasicrystals. The latter are quite fragile, and while using coatings their rigidity is manifested. Another way to avoid the problem of the fragility of the quasicrystalline materials is to use icosahedral quasicrystalline particles of nanometer sizes for the reinforcement of aluminum-based alloys.

Thus, a new state of matter is found that has the long-range order but does not have translational symmetry and has the symmetry elements prohibited for crystals. This state was termed quasicrystalline and it was found for several hundreds of substances, and in all cases these are metal alloys. As well as there are colloid systems. You will never see quasicrystals from the ones known now: for example, there is none of them in ionic substance such as sodium chloride. The oxides, sulfides, sulfates, and so on have no such quasicrystals. These are always metal alloys, often the ones based on aluminum. Why?

Another feature of quasicrystals is that their chemical formulas which are very strange. For example, $Al_{86}Mn_{14}$, i. e., it is not AlMn, not $AlMn_2$, but very strange, outlandish proportions of the chemical elements.

So, how to understand the existence, how to describe the structure of this kind of substance? It is clear today that it is possible to describe the quasicrystals structure in two different ways. The first one is the Penrose tiling which is a classic example of the two-dimensional quasicrystal [4], the second one is a multidimensional description [5].

In 1976, Penrose created a non-periodic tiling of two tiles, thickened and waisted diamonds with strictly defined proportions, and not just simple proportions but the proportions of "the golden ratio" or 1.618... The plane without inconsistencies can be surfaced with two kinds of diamonds: with acute corners of 36 and 72 degrees. The angles of these diamonds are related to the golden ratio. The ratio of the quantity of wide diamonds to the narrow ones is equal to the golden ratio. Since this is an irrational number, it is impossible to separate a lattice cell which would contain a whole number of diamonds. If the node points are replaced with atoms, the Penrose tiling would be a good analogue of the two-dimensional quasicrystal since it has a lot of properties typical for this state of matter.

Firstly, it is possible to separate in the tiling regular polygons having quite similar orientation. They create the long-range orientation order called quasiperiodic. This means that between distant tiling structures there is interaction coordinating the location and the relative orientation of the diamonds in a quite determined though an ambiguous way.

Secondly, if all diamonds with the sides parallel to any chosen direction are consequently painted, they form a series of zigzag lines. Along these zigzag lines it is possible to draw parallel straights distant approximately at the same distance from each other. Due to this property we can speak about some translation symmetry in the Penrose tiling.

Thirdly, consequently painted diamonds form five families of similar parallel lines intersecting at the angles that are multiples of 72°. The directions of these zigzag lines correspond to the directions of the sides of the regular pentagon. Therefore the Penrose tiling has to some extent rotational symmetry of the fifth order and in this sense it is similar to the quasicrystal.

The higher-dimensional approach is based on the information on intensity distribution in the reciprocal space, i. e. it can be applied directly to describe the experimental diffraction data. It is based on the fact that from mathematical point of view the construction of an aperiodic function can be reduced to the sum of harmonic functions with the number of linearly independent wave vectors greater than dimension of the real space. Quasiperiodic functions in s-dimensional space can be considered as irrational sections of n-dimensional periodic functions ($n > s$), where n specifies the minimum dimension of the space of embeddings, and s — dimension of the quasicrystal itself. The structure factor of the quasicrystal in the higher-dimensional approach is calculated based on distribution of hyperatoms in the lattice cell of the n-dimensional lattice. The method allowed classifying the possible symmetry point groups of the axial quasicrystals, setting the dimension of the space of embeddings and corresponding n-dimensional space groups for each case [6, 7].

Matrix models

In 2014, N.Balonin hypothesized: each quasicrystal has corresponding quasiorthogonal matrix associated with it, the golden ratio matrix meets the D.Shechtman quasicrystal.

Let's list some definitions of the matrix theory.

Definition 1. Values, to which elements of the matrix are equal, will be called its *levels*. Thus the Hadamard matrix with elements {1, -1} has two levels (two-level matrix) and the Belevitch matrix (**C**-matrix, conference matrix) with elements {0, 1, -1} is a the three-level one.

Definition 2. Quasiorthogonal will be called a square matrix **A**, order n, with the maximum of the absolute values of its elements reduced to 1, obeying the quadratic equation

$$\boldsymbol{A^T A} = \omega \boldsymbol{I},$$

where **I** — identity matrix; ω — weight of the matrix.

Basically, quasiorthogonal in the broad sense of the word could be called any orthogonal by columns (or rows) matrices. In this case, they would have included orthogonal ones with the weight $\omega = 1$ and the maximum modulus element $m < 1$. However, in this case we are interested in the

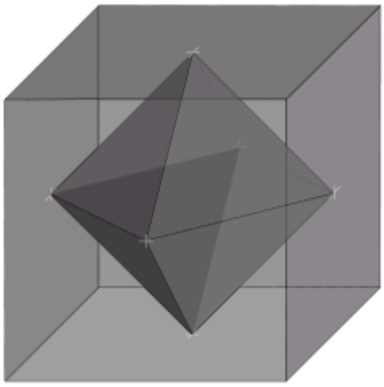

Fig. 1. Octahedron in a cube.

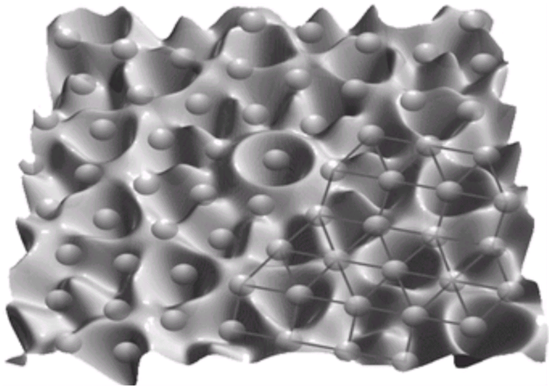

Fig. 2. Microparticles in the field cells.

matrices extreme as for the determinant with restrictions to the values of their elements: they must not be greater than 1. It is obvious that with elementary multiplication by $1/m$ any orthogonal matrix with the determinant equal to 1 is reduced to the quasiorthogonal one, and its determinant increases by $1/m^n$ times.

A further increase of the determinant by scaling is not possible, as this will make the matrix elements larger than 1. From $\det(A)^2 = \omega_n$ and $|\det(A)| = 1/m^n$ follows that $\omega = 1/m^2$.

Geometric interpretation of the matrix determinant is related to volume of the body built on the column-vectors of the matrix. It is a direct way to wording of the close packing problems. For example, in three-dimensional case three orthogonal between themselves ordinary along the length of the column-vectors of the orthogonal matrix represent axis leading to the apexes of an octahedron (they define its position). Let us assume now that the octahedron is in a cube with the coordinates of the apexes equal to 1 or −1.

It is quite obvious that position of the octahedron shown in Fig. 1 is not optimal in terms of its volume. Inclining the octahedron, we deprive it of the contact with the limitation walls and consequently we can increase its volume by scaling. The question is what the optimal position of the expanding octahedron is in which it would be impossible to increase its volume with any turns. This purely geometric problem is also equivalent to the search for the optimal position of the antitank hedgehog for which it is possible to construct a minimal barn. I.e., the same geometric object can occupy larger or smaller volume; it all depends on its position.

Let us now recall that the volume of the octahedron is equal to the determinant of quasiorthogonal matrix. This implies that extreme quasiorthogonal matrices describe the exact solutions of the close packing problems.

The close packing problems also include physical problems of microparticles distribution in the cells of the force field, see Fig. 2. An example is the positions of magnetized needles in the magnetic field. The needles tend to hold not any position but a compact one in terms of their orientation along the force lines.

Geometrical, physical and abstract mathematical models such as the octahedron in confined spaces may have very little in common between themselves. However, let us remember that the Mendeleev table of chemical elements is based on the principle obeyed by the quasiorthogonal matrices as well. In particular, the well-known period of the table corresponds to the contiguity of the forth order of so-called Hadamard matrices — the quasiorthogonal matrices with elements 1 and −1.

With increase of n order the extreme matrices behave quite exotic. In particular, if the order of the matrix is not a multiple of 4, only a part of the elements reaches the values of 1 and -1. The other elements are not equal to the values as large in respect of amplitude, but they are equal among themselves. In other words, the extreme quasiorthogonal matrices are few-level.

The maximum element m of the orthogonal matrix associated with it, of the matrix from which they are obtained by scaling, is called their m-norm; m-norm parameter of the extreme solutions is minimal. In fact, $|\det(A)| = 1/m^n$, the less m value is, the higher determinant is. Consequently, the minimax matrices, orthogonal matrices of the preassigned order with minimal maximum modulus element, correspond to them.

With increase of the odd order n the number of matrices levels increases line-

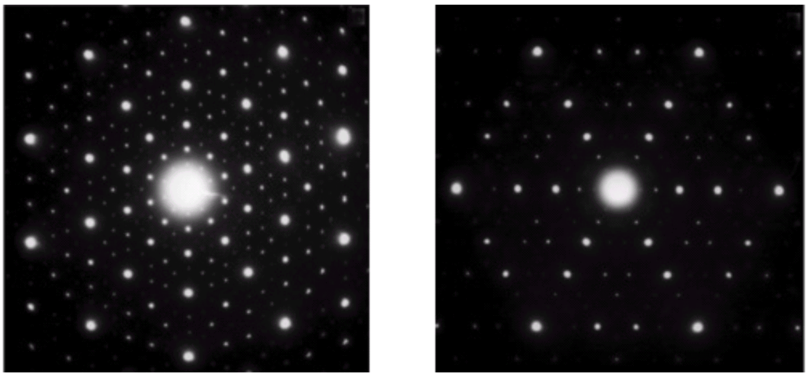

Fig. 3. Diffraction of the Shechtman quasicrystal and of the ordinary crystal.

arly, resembling the bifurcation (splitting of the levels) in chaotic problems. There is also a critical order 13 in which the number of levels increases explosively. It would seem that with this special aspects of extreme problems come to the end. But here we reach the central point of our research. As it is known, the extremums are of two kinds — global (absolute) and local (relative) ones.

It turns out that the behavior of the local extremum matrices, i.e., if we are not interested in the higher determinant value, but still in the extreme one, such suboptimal matrices of the determinant local maximum remain few-level. Moreover, these are often two-level matrices with the elements having values of 1 and $-b$.

Why is this so important?

Because the non-periodic Penrose tiling described as a model of the Shechtman quasicrystal, is the two-dimensional model. Meanwhile, the physical problem is the three-dimensional problem. Figure 3 shows: on the left — diffraction from the quasicrystal along the symmetry axis of the fifth order, and on the right — ordinary diffraction from the crystal with the allowed symmetry of the sixth order.

Let us now imagine that there is the quasiorthogonal matrix of order 10 with the elements 1 and $-b$, $b = 0.618$ .. is one of the numbers of the golden ratio. The matrices of this class, firstly, have never been compared with quasicrystals before; secondly, its level value is hardly casual.

We have now before us a new *ten-dimensional* abstract mathematical model of the Shechtman quasicrystal, and it is important to emphasize that this model generally speaking is not static (as the Penrose model). We will describe it more in details below, but in the meantime we should note

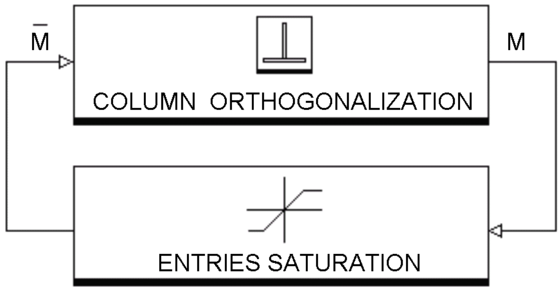

Fig. 4. The matrix search procedure.

that the matrices of the determinant local maximum are natural products of recursive optimization procedures, as well as the quasicrystal is a product of "iterations" of the similar, but the physical nature. In addition to the identity (of some of the features, of course) of the resulting objects there also exists an identity in the behavior leading to the procedures results.

Quasicrystals are products of the very extreme conditions, they are obtained by ultra-fast cooling.

The quasiorthogonal golden ratio matrix with levels 1 and $-b$, $b = 0.618...$ is also a product of specific process. On order 10 the determinant global maximum among quasiorthogonal matrices is observed in **C**-matrix — a matrix with elements 1, -1 (and zero on the diagonal). This matrix has nothing to do with the golden ratio, and the iteration procedure shown in Fig. 4 leads to it. Any non-orthogonal matrix **M** (non-orthogonality is marked with an over-bar) is orthogonalized, for example, with the Gram-Schmidt algorithm. Furthermore, since we are interested in increase of the matrix determinant and it is inversely proportional to degree of the maximum element value, the matrix saturates (quite ordinary nonlinear operation). Looped, this process leads to the determinant extremum of the quasiorthogonal matrix.

In order the extremum was not global but local, it is necessary to change the saturation function, to increase dramatically, for example, small elements, see Fig. 5. We cannot say that this is what models heating of the substance, but we can avoid a matrix with zero elements with this. Hysteresis can be added if required.

Thus, from the static model we arrived at the dynamic model, the one that is studied by the theory of dynamic systems. The matrix on return of this system is an attractor, a condition which is obtained after the dynamic process comes to the end. The parameter leading to bifurcations, i.e. to the increase of the number of levels, is quite specific. This is the matrix order. In large, this is a quadratic problem since we are talking about optimizing the determinant on the quadratic constraint equation.

The bottom of the saturation function (area in the vicinity of 0) in the process of the matrix search forms a kind of "numeric fountains", numbers flows rising up in the matrix. The more intensive process is, the more chances we have to obtain a model of the physical phenomenon that Shechtman obtained with the sharp freezing. And we can "turn off" (freeze) our model at any stage.

The Penrose model is two-dimensional, static and well studied by now. These quasiorthogonal matrices and dynamic processes generating them are quite a different story. These are new models, and we encourage studying them because the findings can be made at the interdisciplinary confluence (the Penrose model was required for understanding the physical result of D.Shechtman).

It is quite obvious that except root of 5 leading to the golden ratio, in these problems associated with the matrices of different orders, we can find any irrationalities built on the roots of the prime numbers: 2, 3, 5, 7, etc. The Shechtman quasicrystal is emphasized by belonging to the class of problems in which the golden ratio is encountered. Other quasicrystals may be well associated with other quasiorthogonal matrices. Are the dynamic processes giving rise to quasiorthogonal matrix, predicting? It may be. After all, the matrix with the level of 0.618... was found.

The number τ (the golden ratio) is a representative of the special class of irrational numbers called algebraic integers. The latter are defined as the roots of the algebraic equation

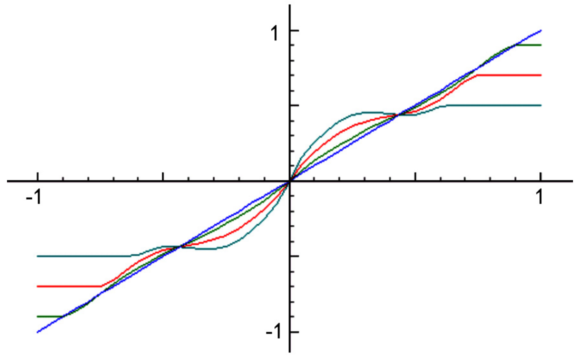

Fig. 5. Different saturation functions.

$$x^n + a_{n-1}x^{n-1} + \ldots + a_0 = 0,$$

where all a_n are integers.

The number τ is determined as a solution of the simplest quadratic equation $\tau^2 = \tau + 1$, which is the self-similarity equation. Writing it in the form of $1 = 1/\tau + 1/\tau^2$, we see that it defines the division of a unit length in two intervals with the lengths of $1/\tau$ and $1/\tau^2$ proportional ratio of which is $\tau = (1 + \sqrt{5})/2 = 1.618$. As for the self-similarity, it is a kind of the symmetry characteristic of the system towards the uniform extension of the system size (scale invariance or scaling). The self-similarity of quasicrystals (and crystals, naturally) consists in the fact that there are points in space towards which with increasing extension to any other point of the lattice by q times, we get back to the lattice point again. Quasicrystals with symmetry of the 5^{th} and the 10^{th} order are self-similar with regard to stretching by τ times, i. e., the golden ratio matrix meets the icosahedral quasicrystal. Presumably, in quasicrystals with symmetry of the 8^{th} and 12^{th} order the coefficients of the self-similarity stretching are $\xi = (1 + \sqrt{2}/2 = 1.207$ and $\psi = (2 + \sqrt{3})/2 = 1.866$, respectively [3].

The numbers τ, ξ, ψ are irrational. The matrices with irrational levels are relatively new objects [10, 11]. To find them, an algorithm of the "tapped" determinant described above is used. Except the golden ratio matrices of the 5^{th} and the 10^{th} orders, there are other matrices of small orders (for example, the Pythagoras matrix) with other irrational numbers-levels corresponding probably to the properties of the existing quasicrystals line.

The golden ratio matrix $\mathbf{G}_{10}$ is a modular two-level matrix with modules of the level a

= 1 and $g = 618...$, it is shown in Fig. 6. Brightness of the cell reflects the value of its element level in the range from 0 (white) to 1 (black); as we can see, the levels are discrete. Golden ratio matrix aspect depends on sorting of the rows and columns, there is a bicyclic shape, but we prefer to present the one in which the oscillations of element signs of the matrix are more clearly visible. Cyclic and bicyclic forms are comparable with the models in which long-range orderliness can be seen, as it takes place with the lines of the magnetic field, whose distant models cyclic matrices are (a combination of chaos in the elements signs along the rows and the rigid orderliness along "diagonals"). The branch of the golden ratio matrices is defined in the orders $n = 10{\cdot}2^k$. The following construction logic is correct for them (similar to the construction logic of the Hadamard matrices): the matrix $\mathbf{G}_{10}$ is the start for the entire sequence of matrices found by iterations represented in the form $\mathbf{G}_{nk} = \begin{bmatrix} G_{nk} & G_{nk} \\ G_{nk} & -G_{nk} \end{bmatrix}$. The function value of the level of these branch matrices is the constant $g = 1/\tau$.

Fig. 6. Golden ratio matrix $\mathbf{G}_{10}$.

4. Conclusions

The field of application of mathematical models in the form of compact in the precise mathematical sense basis is large [9]. For the ordered structures consisting of two endlessly recurring units, the modular two-level golden ratio matrix may be a model reflecting the structure elements. We can find here the same particularities of the problem to be solved — dichotomy of the elements related to the golden ratio. The interest consists not so much in the statement of this, surely, important dependence, but in indication of the prospects: both the materials and the matrices can have different types, in addition to the well-known ones, and the second ones may be involved in predicting the existence and then in analyzing the first ones. The dynamic model is new, it points to a useful link with the theory of dynamical systems, linear operators, random attractors, etc. with their mathematical tools so necessary in the development of views on quasicrystals.

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