

数学と化学の学際共同研究と福井プロジェクト VI

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Mathematics and Chemistry

Interdisciplinary Joint Research and the Fukui Project VI

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This is the sixth part of the series of articles that records and further develops essentials of the Mathematics and Chemistry Interdisciplinary Symposium 2013 Tsuyama, whose main themes were symmetry, periodicity, and repetition. The symposium was held on April 5th and 6th in Tsuyama city, Okayama, Japan, in conjunction with the Fukui Project and was devoted to the memory of the late Professor Kenichi Fukui (1981 Nobel Prize) who initiated the project. The present series also provides challenging cross-disciplinary problems which are directly related to the Fukui conjecture and to recent carbon nanotube research. Most of these problems are formulated using mathematical language of unique factorization domain (UFD) and related notions, which are not well known among chemists despite the importance of these notions in elucidating additivity and high-speed asymptotic phenomena in molecules having many repeating identical moieties.

Key Words: the Fukui conjecture, Memoir of Prof. K. Fukui, Unique factorization domain (UFD), Carbon nanotube, Polyacetylene

7. Answers to Questions of Professor Arimoto Related to Fukui Conjecture

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ABSTRACT. We show that certain ring of real functions on the interval $[0, 2\pi]$ is a Dedekind domain, but not a unique factorization domain (UFD). The problem arose in a study of the Fukui Conjecture and the chemistry of carbon nanotubes.

1. INTRODUCTION

Professor Shigeru Arimoto, in a correspondence to the author dated at July 7, 2014, asked the following two questions, which arose in connection with the Fukui Conjecture and the chemistry of carbon nanotubes (see Arimoto 1), Arimoto-Spivakovsky-Amini-LeBlanc-Taylor-Yoshida-Yokotani-Yamabe 2)-4)).

In the present note, we first recall the questions of Arimoto, then give answers on a broad basis, independently of specific applications.

Let $I = [0, 2\pi]$ be a real interval and let $C^\omega(I)$ be the ring of real analytic functions on I , (see Def. I, Note 1 in Sect. 8 for details of $C^\omega(I)$). Let us consider the subring:

$$C_0^\omega(I) := \{f \in C^\omega(I) : \exists g \in \mathbb{R}[x, y] \\ \text{s.t. } f(\theta) = g(\cos(\theta), \sin(\theta))\}.$$

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Question 1. The ring $C_0^\omega(I)$ may conjecturally not be a UFD. Is this true?

Question 2. Can one transplant the degree function on the ring $\mathbb{R}[x, y]$ to the ring $C_0^\omega(I)$?

2. AN ANSWER TO QUESTION 1

In the following two propositions, we explain the proof.

Proposition 2.1. *The correspondence $g \mapsto f$ in the definition of $C_0^\omega(I)$ induces an isomorphism*

$$\mathbb{R}[x, y] / (x^2 + y^2 - 1) \simeq C_0^\omega(I)$$

of the rings.

Proof. The correspondence $g \mapsto f$ is obviously a surjective ring homomorphism. Clearly, $x^2 + y^2 - 1$ is an element in the kernel of the homomorphism. Let $P \in \mathbb{R}[x, y]$ be an arbitrary element in the kernel of the homomorphism. Regarding P as a polynomial in x , we apply the Euclid division algorithm (Division theorem). Namely, we divide P by $x^2 + y^2 - 1$ as polynomials in x and obtain the quotient A and the residues B and C in the following expression

$$P(x, y) = A(x, y)(x^2 + y^2 - 1) + B(y)x + C(y) \quad (1)$$

for some $A \in \mathbb{R}[x, y]$ and $B, C \in \mathbb{R}[y]$. Suppose $B \neq 0$. Then, $B(\cos(\theta))$ cannot be identically zero (since a polynomial B can have only finite number of roots, but $\cos(\theta)$ takes infinitely many values. On the other hand, applying to (1) the fact that P belongs to the kernel of the homomorphism, one gets a relation

$$B(\cos(\theta)) \cdot \sin(\theta) + C(\cos(\theta)) = 0.$$

This implies the relation

$$\sin(\theta) = -C(\cos(\theta)) / B(\cos(\theta))$$

for θ in I , but it is clear (by analytic continuation) that the relation holds for all real value $\theta \in \mathbb{R}$. This is a contradiction, since the left hand side is a nonzero odd function and the right hand side is an even function. Thus $B(y) = 0$. Again, applying to (1) the fact that P belongs to the kernel, we obtain $C(\cos(\theta)) = 0$. This implies $C = 0$ for the same reason as before. This completes a proof. $\square$

As a consequence of the proposition, the ring $C_0^\omega(I)$ is

isomorphic to a ring of an irreducible affine algebraic curve $x^2 + y^2 - 1 = 0$ over the real number field. In general such ring of regular functions on an affine algebraic curve is well-known to be a Dedekind domain, where any ideal is uniquely decomposes into a product of prime ideals. It is also well-known that a Dedekind domain is a unique factorization domain if and only if its any (prime) ideal is generated by a single element 5), 6). If the coefficient field is the complex number field, then any prime ideal can be generated by a single element, that is, the unique factorization can be shown. For instance, over the complex number field, we have the decomposition

$$x^2 + y^2 = (x + \sqrt{-1}y)(x - \sqrt{-1}y).$$

Then, putting $u = x + \sqrt{-1}y$, we have

$$u^{-1} = x - \sqrt{-1}y$$

in the ring $\mathbb{C}[x, y] / (x^2 + y^2 - 1)$. Therefore, we have

$$\mathbb{C}[x, y] / (x^2 + y^2 - 1) \simeq \mathbb{C}[u, u^{-1}]$$

which is easily seen to be a UFD (since any element is uniquely decomposed into a form $c \prod \frac{(u - a_i)}{(u - b_j)}$ for suitable

$a_i, b_j, c \in \mathbb{C}$ such that there is no pair (i, j) with $a_i = b_j$). However, over the real number field, not all prime are generated by single element so that the ring is not a unique factorization domain. Let us confirm this fact explicitly for the ring of the curve $x^2 + y^2 - 1 = 0$.

Proposition 2.2. *The ring $\mathbb{R}[x, y] / (x^2 + y^2 - 1)$ is not a unique factorization domain. More precisely, the ideal $(x, y - 1)$ is not singly generated.*

Proof. We first note that x is an irreducible element in

$\mathbb{R}[x, y] / (x^2 + y^2 - 1)$. Actually, in

$\mathbb{C}[x, y] / (x^2 + y^2 - 1)$, x decomposes as

$$(u + u^{-1}) / 2 = (u + \sqrt{-1})(u - \sqrt{-1}) / 2u$$

where u is a generator of the units of the ring. Therefore, if x decomposes into a product of non-unit elements in $\mathbb{R}[x, y] / (x^2 + y^2 - 1)$, then each factor should be a unit multiple of $u \pm \sqrt{-1}$. However, this is impossible, since any unit of the ring is of the form cu^m for a non-zero constant $c \in \mathbb{C}$ and an integer $m \in \mathbb{Z}$. But it may be clear that no element of the form $cu^m(u \pm \sqrt{-1})$ can belong to the real coefficient subring

$\mathbb{R}[x, y] / (x^2 + y^2 - 1)$. That is, x is irreducible.

Suppose the ideal $(x, y - 1)$ is generated by single element, then the generator should divide x and $y - 1$. So, irreducibility of x implies that x may be the generator, and that x divides $y - 1$. The last relation can be expressed in terms of the $\mathbb{R}[x, y]$ that there exists polynomials $A, B \in \mathbb{R}[x, y]$ such that

$$x \cdot A(x, y) + B(x, y)(x^2 + y^2 - 1) = y - 1. \quad (2)$$

Substituting $x = 0$ in the relation, one obtains

$$B(0, y)(y^2 - 1) = y - 1$$

in $\mathbb{R}[y]$. This is impossible, since the left hand side can be either identically 0 or a nonzero polynomial in y of degree at least 2. Thus, the ideal $(x, y - 1)$ is not generated by a single element. $\square$

3. TWO ANSWERS TO QUESTION 2

Question 2 itself is generic and the answer depends on what is meant by “degree function”, and on what applications are in one’s mind. In the knowledge of the author, there is not an immediate transplant of the degree function from $\mathbb{R}[x, y]$ to $\mathbb{R}[x, y] / (x^2 + y^2 - 1)$ in a naive sense. Here, we have two possible suggestions of completely different nature. What I write below are general answers independent of any specified applications.

1. Remember the following inclusion map

$$\begin{aligned} & \mathbb{R}[x, y] / (x^2 + y^2 - 1) \\ & \subset \mathbb{C}[x, y] / (x^2 + y^2 - 1) \simeq \mathbb{C}[u, u^{-1}] \end{aligned}$$

where the right hand side is the ring of Laurent polynomials in $u := x + \sqrt{-1}y$. Then, we can talk about whether some element is homogeneous of degree $n \in \mathbb{Z}$ in the variable u , i.e. those elements of the form cu^n ($c \in \mathbb{C}$) where n may be also negative. Then, for a non-negative integer d , define

$$\begin{aligned} \mathbb{C}[u, u^{-1}]_{\leq d} &:= \text{the linear combination of elements} \\ & \text{of degree } n \text{ s.t. } |n| \leq d \\ &= \mathbb{C}u^{-d} + \mathbb{C}u^{-d+1} + \cdots + \mathbb{C}u^{-1} \\ &+ \mathbb{C} + \mathbb{C}u + \cdots + \mathbb{C}u^{d-1} + \mathbb{C}u^d. \end{aligned}$$

Then, we further can consider the subspace

$$\begin{aligned} & (\mathbb{R}[x, y] / (x^2 + y^2 - 1))_{\leq d} \\ &:= (\mathbb{R}[x, y] / (x^2 + y^2 - 1)) \cap \mathbb{C}[u, u^{-1}]_{\leq d}. \end{aligned}$$

So, using $C_0^\omega(I) \simeq \mathbb{R}[x, y] / (x^2 + y^2 - 1)$, we can define the corresponding subspace

$$C_{0, \leq d}^\omega(I) \subset C_0^\omega(I).$$

This space seems to be close to the intended applications.

2. In algebraic geometry, degree of a line bundle means the first Chern class, which can be counted by the number of the zeros of its section. Therefore, over the affine algebraic curve $x^2 + y^2 = 1$, one can introduce the following degree function on $\mathbb{R}[x, y] / (x^2 + y^2 - 1)$ as follows:

$$\deg : \mathbb{R}[x, y] / (x^2 + y^2 - 1) \rightarrow \mathbb{Z}_{\geq 0},$$

$$g \mapsto \dim_{\mathbb{R}} \mathbb{R}[x, y] / (g, x^2 + y^2 - 1).$$

But this number does not satisfy the usual properties, expected for the degree operator so that the author is not sure whether this approach has a meaning.

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8. Challenging Cross-disciplinary Problems Related to the Fukui Conjecture and to the Chemistry of Carbon Nanotubes II

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This is the direct continuation of section 3 of the preceding part IV of this series of papers.

In this section, let $\mathbb{Z}^+$ and $\mathbb{R}$ denote respectively the set of all positive integers and real numbers. In what follows, we retain the notation given in the “Nanotube Series, parts I ~ III” published in the Journal of Mathematical Chemistry^{(1)–(3)}. The reader is referred to refs. 4)–7) for cross-disciplinary investigations related to the Fukui Conjecture and to the chemistry of carbon nanotubes. The reader is also referred to refs. 8)–16) and references therein for the science and technology of carbon nanotubes.

Definitions I. Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. A real-valued function on a subset $S \subset \mathbb{R}$ is called *real analytic* on S if it is the restriction to S of a function which is real analytic on some open set $O \supset S$.

$C^\omega(I)$: the unique factorization domain (UFD) of all real analytic functions defined on I .

[**Note 1:** If $a, b \in \mathbb{R}$ with $a < b$ and if $I = [a, b]$, the unique factorization domain $C^\omega(I)$ can be equivalently and more practically defined by the following:

$$C^\omega(I) = \{f|_I : \exists \varepsilon > 0 \text{ s.t. } f \text{ is real analytic} \\ \text{on an open interval } (a - \varepsilon, b + \varepsilon)\},$$

where $f|_I$ denotes the restriction of the function f to the closed interval I .

It is essential that I is a compact interval for the ring $C^\omega(I)$ to be a UFD. Notice that $f \in C^\omega(I)$ implies that the set of zeroes of f on the compact interval I is, either the whole domain I , or a finite subset of I . In the latter case, observe that f is factored uniquely into irreducible linear terms as follows:

$$f(\theta) = u(\theta) \prod_{j=1}^n (\theta - \theta_j)^{m_j},$$

where u is a unit in $C^\omega(I)$, i.e., u is an invertible function real analytic and with no zeroes on I , $\{\theta_1, \theta_2, \dots, \theta_n\}$ is the finite set of zeroes of f on I , and $m_j \in \mathbb{Z}^+$.

The idea of using the unique factorization domain $C^\omega(I)$ for the proof of the Piecewise Monotone Lemma (PML) [cf. ref. 17) and references therein] dates back to the 1980s and this idea together with the concrete idea for proving the PML via UFDs is due to Professor Kyoji Saito, then the Research Institute for Mathematical Sciences (RIMS), Kyoto University. All versions of the Asymptotic Linearity Theorems, from which the validity of the Fukui conjecture immediately follows, have needed one of several versions of PMLs. See refs. 17)–21) for details. One of the authors of this section (S.A.) expresses his sincere thanks to Professor Kyoji Saito, Professor Isao Naruki, and Professor Mark Spivakovsky, at RIMS in the 1980s, who provided him with PMLs.]

$C^\omega(I)[\lambda]$: the polynomial ring (UFD) over $C^\omega(I)$ in the indeterminate λ .

$\mathbb{R}[\lambda]$: the polynomial ring (UFD) over $\mathbb{R}$ in the indeterminate λ .

$\mathbb{R}[x_1, x_2]$: the polynomial ring (UFD) over $\mathbb{R}$ in the indeterminates x_1, x_2 .

$C_0^\omega(I)$: the subring of $C^\omega(I)$ defined by

$$C_0^\omega(I) := \{f \in C^\omega(I) : \exists g \in \mathbb{R}[x_1, x_2]$$

$$\text{such that } \forall x \in I \quad f(x) = g(\cos x, \sin x)\}.$$

$C_0^\omega(I)[\lambda]$: the polynomial ring over $C_0^\omega(I)$ in the indeterminate λ .

The following is a pedagogical proposition, which is related to the proof of the Fukui conjecture. This proposition and analogous propositions have been introduced in a Challenging seminar for the third graders in Tsuyama National College of Technology (TNCT) in conjunction with a Fourier (frequency) analysis of various sound data. It is not difficult to show that any finite Fourier series function defined on $I = [0, 2\pi]$, which is expressed in terms of a linear combination of $\cos n\theta$ and $\sin n\theta$ functions, is an element of $C_0^\omega(I)$. In the Challenging seminar in TNCT, the derivative of a finite Fourier series function f , which is again a finite Fourier series function, was discussed and the monotonicity number of f and the number of zeroes of its derivative f' were explained by using a computer program called “Graphing Calculator” and by referring to the following proposition:

Proposition A. Let $\phi \in \mathbb{R}[x_1, x_2]$ be a polynomial of two

indeterminates x_1 and x_2 with real coefficients. Let $m \in \mathbb{Z}^+$. Suppose that

$$\deg(\phi) \leq m.$$

Then, we have

$$(i) \text{ Card } \{\theta \in [0, 2\pi]: \phi(\cos\theta, \sin\theta) = 0\} \leq 4m.$$

Moreover, if $u(\theta) := \phi(\cos\theta, \sin\theta)$ is an even function, we have

$$(ii) \text{ Card } \{\theta \in [0, 2\pi]: \phi(\cos\theta, \sin\theta) = 0\} \leq 2m.$$

Proof. Part (i): Let v_j be polynomials of indeterminate x with real coefficients such that

$$\phi(x, y) = \sum_{j=0}^m v_j(x) y^j.$$

Then, $\deg(\phi) \leq m$ implies that

$$\deg(v_j) \leq m - j$$

for all $0 \leq j \leq m$.

If m is an odd number and if $m = 2N + 1$, then we have

$$\phi(\cos\theta, \sin\theta) =$$

$$\sum_{j=0}^N v_{2j+1}(\cos\theta) \sin^{2j+1}\theta + \sum_{j=0}^N v_{2j}(\cos\theta) \sin^{2j}\theta$$

$$= (\sin\theta) \left(\sum_{j=0}^N v_{2j+1}(\cos\theta) \sin^{2j}\theta \right) + \sum_{j=0}^N v_{2j}(\cos\theta) \sin^{2j}\theta$$

$$= (\sin\theta) \left(\sum_{j=0}^N v_{2j+1}(\cos\theta) (1 - \cos^2\theta)^j \right) +$$

$$\sum_{j=0}^N v_{2j}(\cos\theta) (1 - \cos^2\theta)^j.$$

Similarly, if m is an even number and if $m = 2N$, then we have

$$\phi(\cos\theta, \sin\theta) =$$

$$\sum_{j=0}^{N-1} v_{2j+1}(\cos\theta) \sin^{2j+1}\theta + \sum_{j=0}^N v_{2j}(\cos\theta) \sin^{2j}\theta$$

$$= (\sin\theta) \left(\sum_{j=0}^{N-1} v_{2j+1}(\cos\theta) \sin^{2j}\theta \right) + \sum_{j=0}^N v_{2j}(\cos\theta) \sin^{2j}\theta$$

$$= (\sin\theta) \left(\sum_{j=0}^N v_{2j+1}(\cos\theta) (1 - \cos^2\theta)^j \right) +$$

$$\sum_{j=0}^N v_{2j}(\cos\theta) (1 - \cos^2\theta)^j.$$

Thus, there are polynomials A and B with real coefficients such that for all $\theta \in [0, 2\pi]$,

$$\phi(\cos\theta, \sin\theta) = (\sin\theta)A(\cos\theta) + B(\cos\theta),$$

and such that

$$\deg(A) \leq m - 1,$$

$$\deg(B) \leq m.$$

Note that

$$\begin{aligned} & \{\theta \in [0, 2\pi]: \phi(\cos\theta, \sin\theta) = 0\} \\ &= \{\theta \in [0, 2\pi]: (\sin\theta)A(\cos\theta) = -B(\cos\theta)\} \\ &\subset \{\theta \in [0, 2\pi]: (1 - \cos^2\theta)(A(\cos\theta))^2 = (B(\cos\theta))^2\}. \end{aligned}$$

Let

$$P(x) = (1 - x^2)A(x)^2 - B(x)^2$$

so that the degree of the polynomial $P(x)$ is less than or equal to $2m$:

$$\deg(P) \leq 2m.$$

Since $\theta \mapsto \cos\theta$ is a bijection on $[0, \pi]$ and $[\pi, 2\pi]$, we see that

$$\text{Card } \{\theta \in [0, \pi]: P(x) = 0\} \leq 2m,$$

$$\text{Card } \{\theta \in [\pi, 2\pi]: P(x) = 0\} \leq 2m,$$

from which the inequality (i) follows.

Part (ii): Suppose that $u(\theta) := \phi(\cos\theta, \sin\theta)$ is an even function with the domain being analytically extended to $\mathbb{R}$. Then, by Part (i), we see that there are polynomials A and B with real coefficients such that for all $\theta \in [0, 2\pi]$,

$$u(\theta) - B(\cos\theta) = (\sin\theta)A(\cos\theta).$$

Notice that the left-hand side is an even function and that the right-hand side is an odd function. The function that is both even and odd is the constant zero function, i.e., the function that vanishes throughout the domain.

Therefore, we have

$$u(\theta) = B(\cos\theta).$$

By the argument in Part (i), we see that the conclusion of Part (ii) is true. $\square$

In what follows we recall a Lemma called Piecewise Monotone Lemma¹⁷⁾⁻²¹⁾, which played an essential role for the proof of the Fukui conjecture. Before recalling this lemma, we need some preparation:

Definitions II. Let S_1 and S_2 be nonempty subsets of $\mathbb{R}$. A function $f: S_1 \rightarrow S_2$ is said to be *nondecreasing* if $x_1 \leq x_2$ implies $f(x_1) \leq f(x_2)$ for all $x_1, x_2 \in S_1$. A function $f: S_1 \rightarrow S_2$ is said to be *nonincreasing* if $x_1 \leq x_2$ implies $f(x_2) \leq f(x_1)$ for all $x_1, x_2 \in S_1$. A function $f: S_1 \rightarrow S_2$ is said to be *monotone* if it is either nondecreasing or nonincreasing.

Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. A function $f: I \rightarrow \mathbb{R}$ is said to be *piecewise monotone* if there exists a finite partition

$$a = x_0 < x_1 < \dots < x_n = b \quad (n \in \mathbb{Z}^+)$$

of the interval I such that the restriction $f|_{[x_{i-1}, x_i]}$ is monotone for all $i \in \{1, \dots, n\}$. In this case, f is said to have n -partition of monotonicity.

If $f: I \rightarrow \mathbb{R}$ is piecewise monotone, let

$\text{Mo}(f) := \min \{n \in \mathbb{Z}^+ : f \text{ has } n\text{-partition of monotonicity}\}.$

The $\text{Mo}(f)$ is called the *monotonicity number* of f .

If $f: I \rightarrow \mathbb{R}$ is not piecewise monotone, let
 $\text{Mo}(f) = \infty$.

$C(I)$: the ring of all real-valued continuous functions defined on I .

$C(I)[\lambda]$: the polynomial ring over $C(I)$ in the indeterminate λ .

For each $\theta \in I$, let $\text{Ev}_\theta: C(I)[\lambda] \rightarrow \mathbb{R}[\lambda]$ be the ring homomorphism defined by

$$\begin{aligned} \text{Ev}_\theta(c_0\lambda^n + c_1\lambda^{n-1} + \dots + c_n) \\ = c_0(\theta)\lambda^n + c_1(\theta)\lambda^{n-1} + \dots + c_n(\theta). \end{aligned}$$

Now, we are ready to recall the Piecewise Monotone Lemma (version 1)¹⁷⁾:

Lemma A (Piecewise Monotone Lemma (PML))

Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. Let $p \in C^\omega(I)[\lambda]$ be a monic polynomial of degree $q \in \mathbb{Z}^+$ given by

$$p = \lambda^q + c_1\lambda^{q-1} + \dots + c_q.$$

Suppose that for any $\theta \in I$, the polynomial

$$\text{Ev}_\theta(p) = \lambda^q + c_1(\theta)\lambda^{q-1} + \dots + c_q(\theta)$$

over the field $\mathbb{R}$ has q real roots, which we denote by $\lambda_1(\theta) \leq \lambda_2(\theta) \leq \dots \leq \lambda_q(\theta)$. Then, all the λ_j 's are piecewise monotone, i.e.,

$$\text{Mo}(\lambda_j) < \infty$$

for all $j \in \{1, \dots, q\}$.

Our challenging cross-disciplinary problems are as follows:

Problem I. Let q and r be positive integers. In the above lemma, assume that $I = [0, 2\pi]$, $p \in C_0^\omega(I)[\lambda]$ and that

(a) there exist $g_1, g_2, \dots, g_q \in \mathbb{R}[x_1, x_2]$ such that for all $j \in \{1, \dots, q\}$,

$$\deg(g_j) \leq r,$$

$$c_j(\theta) = g_j(\cos\theta, \sin\theta) \quad \text{for all } \theta \in I,$$

(b) p is factored into first degree monic polynomials:

$$p = (\lambda - d_1)(\lambda - d_2) \dots (\lambda - d_q),$$

where $d_1, \dots, d_q \in C^{\omega*}(I)$.

Then, our problem is to get an estimate of $\text{Mo}(d_j)$ of the form:

$$\text{For all } j \in \{1, \dots, q\} \quad \text{Mo}(d_j) \leq \mu(q, r),$$

where μ is a constant function of positive integers q and r .

Problem II. Is it possible to streamline statement (a) in the above Problem I by introducing a 'degree function' or its

conceptual analogue to $C_0^\omega(I)$?

Problem III. In the investigations of carbon nanotubes using the repeat space theory, several analytic formulas concerning energy band curves have been obtained. Is it possible to analyze the monotonicity number of these curves without depending on concrete analytic expressions?

Problem IV. The Fukui Project is international, interdisciplinary, and inter-generational. In connection to the inter-generational aspect of the project, we have been utilizing Matrix Art and Math Art as interfacing and heuristic tools for educational and cross-disciplinary communications. These tools have been mainly visual. Can we proceed further to involve music and other forms of audible art for the same purpose of enriching educational and cross-disciplinary communication?

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