

Normed repeat space and its super spaces: fundamental notions for the second generation Fukui project

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Abstract Fukui's DNA problem is a long-range target of the international and interdisciplinary joint project initiated by Kenichi Fukui in 1992, whose underlying motive has been to cultivate a new interdisciplinary region between chemistry and mathematics for a future development of theoretical chemistry. "Can the conductivity and other properties of a single-walled carbon nanotube be analyzed in the setting of a $*$ -algebra equipped with a complete metric?" This metric problem is fundamental to proceed towards a solution of Fukui's DNA problem. To affirmatively solve this metric problem, we establish, here in this paper, the new notion of normed repeat space $\mathcal{X}_r(q, d, p)$. The normed repeat space $\mathcal{X}_r(q, d, p)$ is an intermediate theoretical device to shift from periodic polymers to aperiodic polymers like DNA and RNA in the above-mentioned Fukui Project. The space $\mathcal{X}_r(q, d, p)$ is a Banach algebra for all $1 \leq p \leq \infty$, and $\mathcal{X}_r(q, d, p)$ forms a C^* -algebra for $p=2$. Here, polymer moiety size number q and dimension number d are arbitrarily given positive integers. The generalized repeat space $\mathcal{X}_r^*(q, d)$ is included in the normed repeat space $\mathcal{X}_r(q, d, p)$, which in turn is included in one of its super spaces $\mathcal{X}_B(q, d, p)$ so that aperiodic polymers can be represented and investigated in the setting of this super space $\mathcal{X}_B(q, d, p)$.

Keywords Repeat space theory (RST) · The Fukui conjecture · Additivity and network problems · Banach algebra · C^* -algebra

This article is dedicated to the memory of the late Professors Kenichi Fukui and Haruo Shingu.

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1 Introduction

The repeat space theory [1–8] and its guiding conjecture, the Fukui conjecture (cf. [1–3] and references therein) played a pivotal role in the First Generation Fukui Project. This international and interdisciplinary joint research project, initiated by the late Professor Kenichi Fukui in 1992, entered a new phase in 2007 as the Second Generation Fukui Project.

Fukui’s DNA problem is a long-range target of the (First and Second Generation) Fukui Project, whose underlying motive has been to cultivate a new interdisciplinary region between chemistry and mathematics for a future development of theoretical chemistry. “Can the conductivity and other properties of a single-walled carbon nanotube be analyzed in the setting of a $*$ -algebra equipped with a complete metric?” This metric problem is fundamental to proceed towards the solution of Fukui’s DNA problem. To affirmatively solve this metric problem, we establish, here in this paper, the new notion of normed repeat space $\mathcal{X}_r(q, d, p)$. The normed repeat space $\mathcal{X}_r(q, d, p)$ is an intermediate theoretical device to shift from periodic polymers to aperiodic polymers like DNA and RNA in the Fukui Project. The space $\mathcal{X}_r(q, d, p)$ is a Banach algebra for all $1 \leq p \leq \infty$, and $\mathcal{X}_r(q, d, p)$ forms a C^* -algebra for $p=2$. Here, polymer moiety size number q and dimension number d are arbitrarily given positive integers. The generalized repeat space $\mathcal{X}_r(q, d)$ is included in the normed repeat space $\mathcal{X}_r(q, d, p)$, which in turn is included in one of its super spaces $\mathcal{X}_B(q, d, p)$ so that aperiodic polymers can be represented and investigated within this super space $\mathcal{X}_B(q, d, p)$.

2 Formulation of the problem

The unifying power and vision of the repeat space theory arise from the idea of identifying molecular sequences with a point of a vector space. Before proceeding to the formulation of the problem given below, the reader is invited to briefly review the notion of the generalized repeat space [2, 4]. Recall the fact that the generalized repeat space $\mathcal{X}_r(q, d)$ (defined for the first time in Ref. [4]) is purely algebraic and lacks in metrics although the auxiliary functional space $AC(I)$ associated with $\mathcal{X}_r(q, d)$ does have a metric.

Recall the sequences $\{M^{a,-b,c,d}_N\}_{N \in \mathbb{Z}^+}$ given in theorem 7.1 (I) in [2] that represent carbon nanotubes.

Problem 1 Is it possible to embed the sequence $\{M^{a,-b,c,d}_N\}$ in a Banach algebra or a C^* -algebra?

We shall affirmatively solve this problem 1 by establishing theorem 1, in Sect. 3.

3 Solution of the problem: theorem 1

We retain the notation in refs. [1–3], and we introduce the following new notation.

Let C^n denote the set of all column n -vectors. For each $1 \leq p \leq \infty$, let

$$\|\xi\|_p := \|(\xi_1, \dots, \xi_n)^T\|_p = (|\xi_1|^p + \dots + |\xi_n|^p)^{1/p}. \tag{3.1}$$

Let

$$\|\xi\|_\infty = \|(\xi_1, \dots, \xi_n)^T\|_\infty = \max \{|\xi_i| : 1 \leq i \leq n\}. \tag{3.2}$$

For each positive integer n and $1 \leq p \leq \infty$, let $\text{Mat}(n, p)$ denote the set of all $n \times n$ complex matrices with the norm given by

$$\|A\|_p = \sup\{\|Ax\|_p/\|x\|_p : x \in \mathbb{C}^n \setminus \{0\}\}. \tag{3.3}$$

Fix $(q, d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$ and let $\mathcal{X}(q, d)$ denote the set of all matrix sequences whose N -th term M_N is an arbitrary $qN^d \times qN^d$ complex matrix, $N \in \mathbb{Z}^+$. This set constitutes a $*$ -algebra over the field \mathbb{C} with term-wise addition, scalar multiplication, multiplication

$$\{M_N\} + \{M'_N\} = \{M_N + M'_N\}, \tag{3.4}$$

$$k\{M_N\} = \{kM_N\}, \tag{3.5}$$

$$\{M_N\}\{M'_N\} = \{M_N M'_N\}, \tag{3.6}$$

and involution $(\cdot)^*$: $\mathcal{X}(q, d) \rightarrow \mathcal{X}(q, d)$ defined by

$$\{M_N\}^* = \{M_N^*\}, \tag{3.7}$$

where the $*$ on the right-hand side of (7) denotes the adjoint operation.

For each $q, d \in \mathbb{Z}^+$ and $1 \leq p \leq \infty$, let

$$\mathcal{X}_B(q, d, p) := \{\{M_N\} \in \prod_{N=1}^\infty \text{Mat}(qN^d, p) : \|\{M_N\}\|_p := \sup_N \|M_N\|_p < \infty\}. \tag{3.8}$$

Note that $\mathcal{X}_B(q, d, p)$ forms a $*$ -subalgebra of $\mathcal{X}(q, d)$. We also note that $\mathcal{X}_B(q, d, p)$ forms a Banach algebra for each $1 \leq p \leq \infty$ and a C^* -algebra for $p=2$. The set $\mathcal{X}_B(q, d, p)$ is called the *bounded underlying space* (or *B-space* for short) of type (q, d, p) .

Now recall the definition of the generalized repeat space with size (q, d) , which is denoted by $\mathcal{X}_r(q, d)$. (Cf. [2,4].)

Theorem 1 For each $q, d \in \mathbb{Z}^+$ and $1 \leq p \leq \infty$, we have

$$\mathcal{X}_r(q, d) \subset \mathcal{X}_B(q, d, p). \tag{3.9}$$

Proof By the definition of $\mathcal{X}_r(q, d)$, for the proof of the proposition it suffices to prove that $a_N := \|(P_N^m S_N^k P_N^n) \otimes Q\|_p$ is a bounded sequence, where $m, n \in \mathbb{Z}^d, k \in \{0, 1\}^d$, and $Q \in \mathbf{M}_q(\mathbb{C})$. Let $r(t, u)$ with $1 \leq t, u \leq q$ denote the $q \times q$ matrix with the t th entry 1 and other entries 0, so that

$$Q = \sum_{t=1}^q \sum_{u=1}^q Q_{tu} r(t, u). \tag{3.10}$$

Then,

$$\begin{aligned} a_N &= \left\| \left(P_N^m S_N^k P_N^n \right) \otimes \left(\sum_{t=1}^q \sum_{u=1}^q Q_{tu} r(t, u) \right) \right\|_p \\ &= \left\| \sum_{t=1}^q \sum_{u=1}^q \left(P_N^m S_N^k P_N^n \right) \otimes (Q_{tu} r(t, u)) \right\|_p \\ &= \left\| \sum_{t=1}^q \sum_{u=1}^q Q_{tu} \left(\left(P_N^m S_N^k P_N^n \right) \otimes r(t, u) \right) \right\|_p \\ &\leq \sum_{t=1}^q \sum_{u=1}^q \left\| Q_{tu} \left(\left(P_N^m S_N^k P_N^n \right) \otimes r(t, u) \right) \right\|_p \\ &\leq \sum_{t=1}^q \sum_{u=1}^q |Q_{tu}| \left\| \left(P_N^m S_N^k P_N^n \right) \otimes r(t, u) \right\|_p. \end{aligned} \tag{3.11}$$

Fix any $N \in \mathbb{Z}^+$ and $1 \leq t, u \leq q$, and let

$$Y := \left(P_N^m S_N^k P_N^n \right) \otimes r(t, u). \tag{3.12}$$

Since by the definitions of P_N , S_N^k , and P_N^n , we have

$$P_N^m = \bigotimes_{i=1}^d P_N^{m_i}, \tag{3.13}$$

$$S_N^k = \bigotimes_{i=1}^d S_N^{k_i}, \tag{3.14}$$

$$P_N^n = \bigotimes_{i=1}^d P_N^{n_i}, \tag{3.15}$$

we see that Y is a $qN^d \times qN^d$ matrix whose entry is either 0 or 1. Recall that an $n \times n$ matrix is called a permutation matrix if it is obtained by permuting the columns of the $n \times n$ identity matrix. Let us call a matrix subpermutation matrix if it is obtained by replacing some (or all) of nonzero elements with zeroes in a permutation matrix.

We wish to prove the following

Proposition 1 *The product of two subpermutation matrices is a subpermutation matrix and the Kronecker product of two subpermutation matrices is a subpermutation matrix.*

Proof of proposition 1 Let $A(x)$ and $B(x)$ be matrices with entries either 0, 1, or the variable x , such that $A(1)$ and $B(1)$ are permutation matrices and $A(0)$ and $B(0)$ are

subpermutation matrices. Consider the product $A(x)B(x)$, then we see that the entries are either 0, 1, x , or x^2 . It can be easily seen that $A(1)B(1)$ is a permutation matrix. It easily follows that $A(0)B(0)$ is a subpermutation matrix. Similarly, one verifies that the Kronecker product of two subpermutation matrices is a subpermutation matrix. //

Now by the definitions of P_N and S_N and their exponents, we see that $P_N^{m_i}$ and $S_N^{k_i}$ are subpermutation matrices. (The matrix $P_N^{m_i}$ is a permutation matrix.) Hence, it follows that Y is a $qN^d \times qN^d$ subpermutation matrix. By the definition of the $\|\cdot\|_p$ matrix-norm, it is easily seen that

$$\|Y\|_p \leq 1. \quad (3.16)$$

Hence, the nonnegative sequence a_N is bounded:

$$a_N \leq \sum_{t=1}^q \sum_{u=1}^q |Q_{tu}|. \quad (3.17)$$

This completes the proof of theorem 1.

4 Definition of the normed repeat space and concluding remarks

Definition 1 For each $q, d \in \mathbb{Z}^+$ and $1 \leq p \leq \infty$, let

$$\mathcal{X}_r(q, d, p) := \text{closure of } \mathcal{X}_r(q, d) \subset \mathcal{X}_B(q, d, p). \quad (4.1)$$

The set $\mathcal{X}_r(q, d, p)$ is called the *normed repeat space of type* (q, d, p) .

Note that $\mathcal{X}_r(q, d, p)$ forms a Banach algebra for each $1 \leq p \leq \infty$ and a C^* -algebra for $p=2$. This fact easily follows from the observation that linear operations, multiplication, and involution are all continuous operations and that any closed set in a complete metric space forms a complete metric subspace. (The reader is referred e.g. to refs. [9, 10] for the fundamental properties of Banach algebras and C^* -algebras.)

We remark that the notion of the normed repeat space established here unites the approaches via the aspects of form and general topology exploited in a variety of asymptotic analyses of molecular networks in [1–7] and references therein. Equipped with the machinery of Banach algebras and C^* -algebras, the notion of normed repeat space with the above-mentioned new unifying power forms a basis of the second generation Fukui project. For a review of the first generation Fukui project, whose basic philosophy we would like to carry on to the second generation project, the reader is referred to ref. [8] entitled ‘Note on the repeat space theory—its development and communications with Prof. Kenichi Fukui—’.

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