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Repeat space theory applied to carbon nanotubes and related molecular networks. II*

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The present article is part II of a series devoted to extending the Repeat Space Theory (RST) to apply to carbon nanotubes and related molecular networks. In this part II, three new versions of the Asymptotic Linearity Theorems, which are central in the RST and played a key role in part I of this series, have been established in a new theoretical framework of the generalized repeat space $\mathscr{X}_r(q, d)$. These new versions of theorems, which prove the Fukui conjecture and solve additivity and molecular network problems in a context broader than before, unite the present series and the seven paper series of structural analysis of chemical network systems published in the International Journal of Quantum Chemistry. Along with the Fukui conjecture, which is the guiding conjecture of the RST, the research target of mathematical and computational modeling called the 'virtual nanotube tip RST atomic force microscopy' has been set up in connection with a variety of modern microscopy useful for nanoscience and technology.

KEY WORDS: repeat space theory (RST), asymptotic linearity theorem (ALT), additivity and network problems, $*$-algebra, the Fukui conjecture, carbon nanotubes, algebraic and analytic curves, resolution of singularities, virtual nanotube tip RST atomic force microscopy

AMS subject classification: 92E10, 15A18, 46E15, 13G05, 14H20

1. Introduction

Hybrid methodology of the repeat space theory (RST) and Kenichi Fukui's reactivity index theory, which is a fundamental part of his celebrated frontier orbital theory, was developed for the first time in parts VI and VII of the seven paper series [1–7] published in the International Journal of Quantum Chemistry. This series is entitled 'Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems

* The present series of articles is closely associated with the series of articles entitled 'Proof of the Fukui conjecture via resolution of singularities and related methods' published in the JOMC.

of Spectral Resolution' and we shall henceforth call it the 'structural analysis series' for short. The above hybrid methodology and associated theoretical tools were formulated in the new language of the generalized repeat space $\mathscr{X}_r(q, d)$. Its definition was first given in [8] by the present author and it has enabled one to handle in a new global context a variety of molecular problems from a unifying perspective.

Part I of the structural analysis series [1] played an important role in applying the RST to carbon nanotubes and monocyclic polyenes in part I of the present series of articles [9] which shall be henceforth called the 'RST-nano series' for short.

Several theoretical links have already been established between the structural analysis series and the RST-nano series. However, we can further achieve the following progress (i)–(iii), if problem 1 given below is affirmatively answered.

(i) The most fundamental core of each series can be theoretically unified,

(ii) the Fukui conjecture (which is the guiding conjecture of the RST; cf. [10] and references therein) is proved on a new powerful basis of the $*$-algebra of the generalized repeat space $\mathscr{X}_r(q, d)$,

(iii) the conductivity of carbon nanotubes and the aromaticity of monocyclic polyenes are illuminated from a unifying perspective of the generalized repeat space $\mathscr{X}_r(q, d)$ in conjunction with the above-mentioned hybrid methodology originating from the RST and the frontier orbital theory.

The generalized repeat space $\mathscr{X}_r(q, d)$ was first defined in [8] by the present author and was exploited in parts V–VII of the structural analysis series [5–7] and in part I of the RST-nano series [9]. The space $\mathscr{X}_r(q, d)$ is a far-reaching d-dimensional generalization of the original repeat space $X_r(q)$, which also was first defined by the present author (cf. section 2 of ref. [10] for the review of the original repeat space $X_r(q)$).

Problem 1. Is it possible to establish the Asymptotic Linearity Theorems (ALTs), which are central in the RST, on the basis of the generalized repeat space $\mathscr{X}_r(q, d)$?

The main purpose of this article is to give an affirmative answer to the above problem 1, which is going to be reformulated explicitly as problem 2 in section 2. The affirmative answer to problem 2 is given in section 4 after some preparation in section 3. In section 5, along with the guideline of the Fukui conjecture, the research target of mathematical and computational modeling called the 'virtual nanotube tip RST atomic force microscopy' is set up in connection with a variety of modern microscopy useful for nanoscience and technology.

2. Formulation of problem 2

We retain the notation in [9,10]. The new notation necessary in this article is given in the following:

Definitions 1. If M is a complex matrix, $\sigma(M)$ denotes the set of all the eigenvalues of M.

Recall the definitions of the generalized repeat space $\mathscr{X}_r(q,d)$ and its underlying space $\mathscr{X}(q,d)$ from [8] or from the appendix of [9]. For each $(q,d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$, define two subsets $\mathscr{X}_H(q,d)$ and $\mathscr{X}_{Hr}(q,d)$ of $\mathscr{X}(q,d)$ by

$$\mathscr{X}_H(q,d) := \{\{M_N\} \in \mathscr{X}(q,d) : {M_N}^* = M_N \text{ for all } N \in \mathbb{Z}^+\}, \tag{2.1}$$

$$\mathscr{X}_{Hr}(q,d) := \mathscr{X}_H(q,d) \cap \mathscr{X}_r(q,d), \tag{2.2}$$

and recall the definition of $\mathscr{X}_\sigma(q,d)$ given in [6]:

$$\mathscr{X}_\sigma(q,d) := \{\{M_N\} \in \mathscr{X}(q,d) : \bigcup_{N \in Z^+} \sigma(M_N) \text{ is a bounded set in } \mathbb{C}\}. \tag{2.3}$$

An element $\{M_N\} \in \mathscr{X}_H(q,d)$ shall be called an *Hermitian element of* $\mathscr{X}(q,d)$.

We remark that by theorem 3 in [6], and by definitions (2.2) and (2.3), we have

$$\mathscr{X}_{Hr}(q,d) \subset \mathscr{X}_r(q,d) \subset \mathscr{X}_\sigma(q,d) \tag{2.4}$$

for all $(q,d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$.

Let $\{M_N\} \in \mathscr{X}_\sigma(q,d)$ and let J be a subset of $\mathbb{C}$, then, as in [6], J is said to be *compatible with* $\{M_N\}$ if

$$\bigcup_{N \in Z^+} \sigma(M_N) \subset J. \tag{2.5}$$

Now we are ready to formulate

Problem 2. Is it possible to upgrade the following theorems 1–3, which were previously proved in the framework of the original repeat space $X_r(q)$ (cf. [10] for the chronological explanation and the mutual relationships of these theorems) to theorems 4–6 given below, which are formulated in terms of the generalized repeat space $\mathscr{X}_r(q,d)$ and are stronger than theorems 1–3, respectively.

Note 1. By the definitions of $X_r(q)$, $\mathscr{X}_r(q,\, d)$, and $\mathscr{X}(q,\, d)$, it is easily seen that for any $q \in \mathbb{Z}^+$ we have

$$X_r(q) \subset \mathscr{X}_{Hr}(q, 1) \subset \mathscr{X}_r(q, 1). \tag{2.6}$$

Whereas the original repeat space $X_r(q)$ has the structure of a Jordan algebra, the generalized repeat space $\mathscr{X}_r(q, d)$ has the structure of an ordinary algebra, which is simpler and more easily handled than a nonassociative Jordan algebra.

Theorem 1 (practical ALT, $X_r(q)$ version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in AC(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.7}$$

as $N \to \infty$.

Theorem 2 (functional ALT, $X_r(q)$ version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, there exist functionals $\alpha, \beta \in AC(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.8}$$

as $N \to \infty$, for all $\varphi \in AC(I)$.

Theorem 3 (polynomial ALT, $X_r(q)$ version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in P(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) \tag{2.9}$$

for all $N \gg 0$.

Theorem 4 (practical ALT, $\mathscr{X}_{Hr}(q, 1)$ version). Let $\{M_N\}$ be a fixed element of $\mathscr{X}_{Hr}(q, 1)$, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in AC(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.10}$$

as $N \to \infty$.

Theorem 5 (functional ALT, $\mathscr{X}_{Hr}(q, 1)$ version). Let $\{M_N\}$ be a fixed element of $\mathscr{X}_{Hr}(q, 1)$, let I be a fixed closed interval compatible with $\{M_N\}$. Then, there exist functionals $\alpha, \beta \in AC(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.11}$$

as $N \to \infty$, for all $\varphi \in AC(I)$.

Theorem 6 (polynomial ALT, $\mathscr{X}_{Hr}(q, 1)$ version). Let $\{M_N\}$ be a fixed element of $\mathscr{X}_{Hr}(q, 1)$, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in P(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\mathrm{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) \tag{2.12}$$

for all $N \gg 0$.

Note 2. Suppose that the matrix M_N in theorem 6 is such that

$$M_N = K_N^{a,b,1,1} \tag{2.13}$$

for all $N \geqslant 2$, where $K_N^{a,b,1,1}$ is given by equation (4.8) in part I of this series of articles [9]. Then, one can consider closed random walks on the molecular graph $\mathrm{Graph}_N^{a,b,1,1}$ associated with nanotube[a, b, 1, 1], and one can infer the relationship (2.12) from the graph theoretical view point. For the fundamentally important notion of random walks on a graph, the reader is referred to Klein et al. [11], Tang et al. [12], Jiang et al. [13], Graovac et al. [14], and Balaban [15] and references therein.

Given an element $\{M_N\}$ in $\mathscr{X}_{Hr}(q, 1)$, say by (2.13), it is both heuristic and pedagogical to observe the pattern of the finite sequence $(\varphi(M_N))_{11}$, $(\varphi(M_N))_{22}$, $(\varphi(M_N))_{33}, \ldots$, for a given function $\varphi \in AC(I)$, or $\varphi \in P(I)$. (One can observe other patterns of the entries $(\varphi(M_N))_{ij}$ of the matrix $\varphi(M_N)$ by suitably imposing a relation between the indices i and j.) This type of matrix pattern can be most effectively and heuristically analyzed by combining

- Numerical calculation,
- Visual representation,
- Audible representation,

of the entries $(\varphi(M_N))_{ij}$, in which the latter two representations are made by using/developing suitable software that converts the numerical results to visual and audible data. This combined form of global matrix pattern analysis in the RST shall be called the Numerical/Visual/Audible pattern analysis, or the NVA pattern analysis for short. The '*audiolization*' of numerical data is particularly effective in the heuristic global pattern recognition in the RST. The details of the NVA pattern analysis shall be published elsewhere.

3. Reduction of problem 2 to a compatibility problem

In this section, we reduce the solution of problem 2 to that of a problem (problem 3) which is called a compatibility problem in the RST (cf. [10]).

First, note that theorem 5 is obviously a stronger form of theorem 4:

$$\text{theorem 5} \;\Rightarrow\; \text{theorem 4}. \tag{3.1}$$

Proof of theorem 4. This is a direct consequence of theorem 5. □

Second, note that the following theorem 7 easily implies theorem 6:

$$\text{theorem 7} \Rightarrow \text{theorem 6}. \tag{3.2}$$

Proof of theorem 6. By theorem 7 and the definition of $\mathscr{X}_r(q,1)$, we see that for any $\varphi \in P(I)$ there exist $\alpha(\varphi)$, $\beta(\varphi) \in \mathbb{C}$ such that (2.12) holds for all $N >> 0$. But, $\mathrm{Tr}\varphi(M_N)$ given in theorem 6 is real for all positive integers N. It then follows that both the imaginary parts of the complex numbers $\alpha(\varphi)$ and $\beta(\varphi)$ vanish. (One can also get the conclusion of theorem 6 directly from theorem 4.2 in part V of the structural analysis series [5], by using the fact that $\mathrm{Tr}\varphi(M_N)$ in theorem 6 is real for all positive integers N and that any Hermitian matrix is normal.) □

Theorem 7 (polynomial closure theorem, $\mathscr{X}_r(q,1)$-$P(I)$ version). Let $\{M_N\} \in \mathscr{X}_r(q,1)$ be a fixed generalized repeat sequence. Let I be a fixed closed interval compatible with $\{M_N\}$. Suppose that $\varphi \in P(I)$, then we have

$$\{\varphi(M_N)\} \in \mathscr{X}_r(q,1). \tag{3.3}$$

Proof. Suppose that $\varphi \in P(I)$ and is given by

$$\varphi(t) = c_0 t^0 + \cdots + c_n t^n, \tag{3.4}$$

where n is a nonnegative integer and $c_0, \ldots, c_n \in \mathbb{R}$. Note that

$$\{\varphi(M_N)\} = \{c_0 M_N^0 + \cdots + c_n M_N^n\} \tag{3.5}$$

and that

$$\{M_N^0\} = \{qN \times qN \text{ unit matrix }\} \in \mathscr{X}_r(q,1). \tag{3.6}$$

Since $\mathscr{X}_r(q,1)$ is a linear space, to show that (3.3) is true, we have only to verify that

$$\{M_N^m\} \in \mathscr{X}_r(q,1) \tag{3.7}$$

for each $m \in \mathbb{Z}^+$. But, (3.7) can be easily proved by induction on m, bearing in mind the fact that $\mathscr{X}_r(q, 1)$ is closed under the product operation defined by

$$\{K_N\}\{L_N\} = \{K_N L_N\}. \tag{3.8}$$

(cf. [5] for details of the closure properties of $\mathscr{X}_r(q, 1)$). □

For the answer to problem 2, we now have only to prove theorem 5. Before proving theorem 5, we need to establish the following theorems 8–10.

Theorem 8 (direct sum theorem, $\mathscr{X}_r(q, 1)$ version). For each $q \in \mathbb{Z}^+$, we have

(i) $\mathscr{X}_{\#\alpha}(q, 1)$ forms a linear subspace of $\mathscr{X}_\alpha(q, 1)$ and of $\mathscr{X}_r(q, 1)$.

(ii) $\mathscr{X}_r(q, 1)$ is the direct sum of its linear subspaces $\mathscr{X}_{\#\alpha}(q, 1)$ and $\mathscr{X}_\beta(q, 1)$:

$$\mathscr{X}_r(q, 1) = \mathscr{X}_{\#\alpha}(q, 1) \dot{+} \mathscr{X}_\beta(q, 1). \tag{3.9}$$

Proof. Recall proposition 6.1 in [10], which is the $X_r(q)$ version of this theorem. We get the conclusion of theorem 8 in the same way as in the proof of proposition 6.1 in [10]. □

Definitions 2. First, let us recall from [9] the definitions of a standard alpha sequence, standard alpha space, and the FS map associated with a standard alpha sequence:

Fix any $q \in \mathbb{Z}^+$, let $\{A_N\} = A_1, A_2, \ldots$ be an infinite sequence of matrices whose Nth term is a $qN \times qN$ complex matrix. Suppose that there exist $v \in \mathbb{Z}_0^+$, $Q_{-v}, Q_{-v+1}, \ldots, Q_v \in \boldsymbol{M}_q(\mathbb{C})$ such that for each $N \in \mathbb{Z}^+$,

$$A_N = \sum_{j=-v}^{v} P_N^j \otimes Q_j. \tag{3.10}$$

Then, $\{A_N\}$ is called a *standard alpha sequence with size* $(q, 1)$. The set of all the standard alpha sequences is referred to as the *standard alpha space with size* $(q, 1)$ and denoted by $\mathscr{X}_{\#\alpha}$ $(q, 1)$.

Let $F\colon \mathbb{R} \to \boldsymbol{M}_q(\mathbb{C})$ be the $q \times q$ complex matrix-valued function defined by

$$F(\theta) = \sum_{j=-v}^{v} (\exp(ij\theta)) Q_j. \tag{3.11}$$

Then, F is called the FS *map associated with the standard alpha sequence* $\{A_N\}$. (Note that F has the form of a finite Fourier series.)

If A_N is Hermitian for all $N \in \mathbb{Z}^+$, then we have

$$Q_{-j} = Q_j^* \tag{3.12}$$

for all $j \in \{0, 1, \dots, v\}$, and it follows that $F(\theta)$ defined by (3.11) is Hermitian for all $\theta \in \mathbb{R}$.

Second, let $\{M_N\} \in \mathscr{X}_r(q, 1)$. Let $\{A_N\} \in \mathscr{X}_{\#\alpha}(q, 1)$ and $\{B_N\} \in \mathscr{X}_\beta(q, 1)$ be the uniquely determined elements of the direct sum $\mathscr{X}_r(q, 1) = \mathscr{X}_{\#\alpha}(q, 1) \dot{+} \mathscr{X}_\beta(q, 1)$ such that

$$\{M_N\} = \{A_N\} + \{B_N\}. \tag{3.13}$$

Let F be the FS map associated with the standard alpha sequence $\{A_N\}$, then F is called the FS *map associated with the sequence* $\{M_N\} \in \mathscr{X}_r(q, 1)$.

Theorem 9 (functional alpha existence theorem, $\mathscr{X}_{Hr}(q, 1) - C(I)$ version). Let $\{M_N\}$ be a fixed element of $\mathscr{X}_{Hr}(q, 1)$, let I be a fixed closed interval compatible with $\{M_N\}$. Then, there exists a functional $\alpha \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ such that

$$\frac{\mathrm{Tr}\varphi(M_N)}{N} = \alpha(\varphi) + o(1) \tag{3.14}$$

as $N \to \infty$, for all $\varphi \in C(I)$.

Proof. Recall theorem 4.5 in [10], which is the $X_r(q)$ version of this theorem. We get the conclusion of theorem 9 in the same way as in the proof of theorem 4.5 in [10]. □

Theorem 10 (functional alpha representation theorem, $\mathscr{X}_{Hr}(q, 1)$-$C(I)$ version). Notation and the assumptions being as in theorem 9, let F be the FS map associated with the sequence $\{M_N\}$ and let $\alpha \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ be such that (3.14) holds. Define the functional $\alpha^{\mathrm{int}} : C(I) \to \mathbb{R}$ by

$$\alpha^{\mathrm{int}}(\varphi) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{Tr}\varphi(F(\theta)) d\theta. \tag{3.15}$$

Then, we have

$$\alpha = \alpha^{\mathrm{int}}. \tag{3.16}$$

Note 3. To see that α^{int} is well-defined in theorem 10, we need a new compatibility theorem given section 4. See note 5 given in section 4.

Proof of theorem 10. First, recall that the Stone–Weierstrass theorem, which implies that the set $P(I)$ of all polynomial functions with real coefficients is a dense subset of $C(I)$:

$$\overline{P(I)} = C(I), \tag{3.17}$$

where $C(I)$ denotes the normed space of all real-valued continuous functions on I equipped with the uniform norm given by

$$||\varphi||_u = \sup\{|\varphi(t)| : t \in I\}. \tag{3.18}$$

It is easy to verify that α^{int} is bounded:

$$\alpha^{\text{int}} \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R}). \tag{3.19}$$

Hence α^{int} is continuous. By the continuity of the functionals α and α^{int}, for the proof of the theorem, we have only show that

$$\alpha(\varphi) = \alpha^{\text{int}}(\varphi) \tag{3.20}$$

for all $\varphi \in P(I)$.

Second, recall (A.13) in the appendix of [9], and notice that if $\{B_N\} \in \mathscr{X}_\beta(q,\ 1)$ then B_N has the following form for all $N \gg 0$:

$$B_N = \begin{pmatrix} W_1 & & W_2 \\ & \mathbf{0} & \\ W_3 & & W_4 \end{pmatrix}, \tag{3.21}$$

where W_1, W_2, W_3, and W_4 are $qw \times qw$ complex matrices, $w \in \mathbb{Z}^+$; and w and W_j are constant and independent of N.

Third, recall proposition 4.5(1)–(4) of [5] reproduced as lemma 1.

Lemma 1. For each $(q,\ d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$ we have:

(1) $\mathscr{X}_\alpha(q, d)\mathscr{X}_\alpha(q, d) \subset \mathscr{X}_\alpha(q, d)$,

(2) $\mathscr{X}_\alpha(q, d)\mathscr{X}_\beta(q, d) \subset \mathscr{X}_\beta(q, d)$,

(3) $\mathscr{X}_\beta(q, d)\mathscr{X}_\alpha(q, d) \subset \mathscr{X}_\beta(q, d)$,

(4) $\mathscr{X}_\beta(q, d)\mathscr{X}_\beta(q, d) \subset \mathscr{X}_\beta(q, d)$.

Fourth, for each nonnegative integer j, let $(\cdot)^j : \mathscr{X}(q,1) \to \mathscr{X}(q,1)$ denote the jth power operation defined by

$$\{K_N\}^j = \{K_N^j\}. \tag{3.22}$$

Now let $\{A_N\} \in \mathscr{X}_{\#\alpha}(q,1)$ and $\{B_N\} \in \mathscr{X}_\beta(q,1)$ be such that (3.13) holds.

By using lemma 1, we see that the following relation holds for any nonnegative integer j:

$$(\{A_N\} + \{B_N\})^j - \{A_N\}^j \in \mathscr{X}_\beta(q,1). \tag{3.23}$$

Thus, for any $\varphi \in P(I)$, recalling the form (3.21), we have

$$\mathrm{Tr}\varphi(M_N) - \mathrm{Tr}\varphi(A_N) = O(1) \tag{3.24}$$

as $N \to \infty$. This obviously implies that for any $\varphi \in P(I)$

$$\frac{\mathrm{Tr}\varphi(M_N)}{N} - \frac{\mathrm{Tr}\varphi(A_N)}{N} = o(1) \tag{3.25}$$

as $N \to \infty$.

Let $\theta \in [0, 2\pi]$ and let $h_j(\theta)$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counting the multiplicity, arranged in the increasing order:

$$h_j(\theta) = \lambda_j(F(\theta)), \tag{3.26}$$

where $j \in \{1, \ldots, q\}$. By using proposition 2.1 in [19], we can easily prove that the function $h_j : [0, 2\pi] \to \mathbb{R}$ defined by (3.26) is continuous for all $j \in \{1, \ldots, q\}$. Note that

$$\frac{1}{2\pi}\int_0^{2\pi} \mathrm{Tr}\varphi(F(\theta))d\theta = \frac{1}{2\pi}\int_0^{2\pi}\sum_{j=1}^{q}\varphi(h_j(\theta))d\theta \tag{3.27}$$

for all $\varphi \in C(I)$. On the other hand, the block-diagonalization formula for a standard alpha sequence, theorem 7.2(ii) in [9], implies that

$$\frac{\mathrm{Tr}\varphi(A_N)}{N} = \frac{1}{N}\sum_{r=1}^{N}\sum_{j=1}^{q}\varphi\left(h_j\left(\frac{2\pi r}{N}\right)\right). \tag{3.28}$$

Notice that for each $\varphi \in C(I)$, the function $\sum_{j=1}^{q}\varphi \circ h_j$ is continuous thus Riemann integrable on [0, 2π]. We now see that for each $\varphi \in C(I)$

$$\frac{\mathrm{Tr}\varphi(A_N)}{N} \to \frac{1}{2\pi}\int_0^{2\pi}\mathrm{Tr}\varphi(F(\theta))d\theta \tag{3.29}$$

as $N \to \infty$. From this and (3.25), we have for each $\varphi \in P(I)$.

$$\frac{\mathrm{Tr}\varphi(M_N)}{N} \to \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Tr}\varphi(F(\theta))d\theta \tag{3.30}$$

as $N \to \infty$, which shows that (3.20) is true for all $\varphi \in P(I)$. □

Now we are ready to provide

Proof of theorem 5. Let $\{A_N\} \in \mathscr{X}_{\#\alpha}(q, 1), \{B_N\} \in \mathscr{X}_{\beta}(q, 1)$ be such that

$$\{M_N\} = \{A_N\} + \{B_N\}. \tag{3.31}$$

Assume that an answer to the following problem is affirmative:

Problem 3. Notation being as above, is I compatible with $\{A_N\}$?

Then, in view of theorems 6, 9, and 10, which we have established in the present article, we see that we can use the same proof method as in the proof of theorem 3.4 of ref. [10] to reach the conclusion of theorem 5. Therefore the proof of theorem 5 (and hence the affirmative solution of problems 1 and 2) is reduced to solving problem 3 affirmatively, which we shall do in section 4.

Note 4. The decomposition of an element $\{M_N\}$ in the (generalized or original) repeat space into an α sequence and a β sequence is a fundamental technique in the RST and it is called the 'α–β sequence decomposition.' We remark that this technique can be applied to the theory of Toeplitz matrices, which has recently turned out to be useful in the investigation of carbon nanotubes. The reader who is interested in applications of this technique to the theory of Toeplitz matrices is referred to Zizler et al. [16] and A. Böttcher and Grudsky's monographs [17,18] which are, respectively entitled:

- Toeplitz Matrices, Asymptotic Linear Algebra, and Functional Analysis,
- Spectral Properties of Banded Toeplitz Matrices.

We also remark that in paper [16], a linkage between

(i) the mathematical study of Toeplitz matrices, and

(ii) the repeat space theory (RST)

has been formed for the first time. Namely, in dealing with Toeplitz matrices in the proof of the main theorem, theorem 2.3 in [16], we have recalled, sharpened, and applied a mathematical technique developed in the RST (to estimate quantum boundary effects in polymeric molecules). It is also remarkable that the sharpened technique in the proof of theorem 2.3 in [16] can be applied to molecular problems by embedding the technique into the RST. In our opinion, researchers investigating in areas of the above (i), (ii), and

(iii) the quantum chemistry of polymers and solids,

(iv) the graph theory related to macromolecules and solids,

can mutually benefit from these connections. The reader who is interested in cross-disciplinary mathematical investigations in chemistry is referred to [4–10,19,20,25] and references therein, where he/she can find the genesis of the RST (in conjunction with experimental chemistry) and a variety of applications of the RST to quantum, thermodynamic, and structural chemistry.

4. Solution of problem 3 via a new compatibility theorem

In this section, we give an affirmative answer to problem 3 by establishing the following theorem 11, which is a generalization of theorem 6.1 (compatibility theorem, $X_r(q)$ version) established in [10].

Theorem 11 (compatibility theorem, $\mathscr{X}_{Hr}(q,1)$ version). Let $\{M_N\} \in \mathscr{X}_{Hr}(q,1)$. Let $\{A_N\} \in \mathscr{X}_{\#\alpha}(q,1)$ be the standard alpha sequence such that $\{M_N\} - \{A_N\} \in \mathscr{X}_{\beta}(q,1)$. Let F be the FS map associated with $\{A_N\}$. Then, we have

(i)
$$\bigcup_{0\leqslant\theta\leqslant 2\pi} \sigma(F(\theta)) = \overline{\bigcup_{N\geqslant 1} \sigma(A_N)}. \tag{4.1}$$

(ii)
$$\bigcup_{0\leqslant\theta\leqslant 2\pi} \sigma(F(\theta)) \subset \overline{\bigcup_{N\geqslant 1} \sigma(M_N)}. \tag{4.2}$$

(iii) Suppose that I is a closed interval compatible with $\{M_N\}$. Then, I is compatible with both $\{A_N\}$ and F.

Proof. Let $\theta \in [0, 2\pi]$ and let $h_j(\theta)$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counting the multiplicity, arranged in the increasing order:

$$h_j(\theta) = \lambda_j(F(\theta)), \tag{4.3}$$

where $j \in \{1,\ldots,q\}$. By using proposition 2.1 in [19], we can easily prove that the function $h_j\colon [0, 2\pi] \to \mathbb{R}$ defined by (4.3) is continuous for all $j \in \{1,\ldots,q\}$. (Recall the same argument of continuity in the proof of theorem 10). The rest of the proof of theorem 11 proceeds in the same way as in the proof of theorem 6.1 (compatibility theorem, $X_r(q)$ version) in [10]. □

Note 5. We remark that theorem 11(iii) implies that α^{int} given in theorem 10 is well-defined.

The proof of the compatibility theorem, $X_r(q)$ version, depended on proposition I in [20], which asserts the Lipschitz continuity of h_j. (Note that the Sturmian separation theorem was used in [20] to prove the Lipschitz continuity of h_j.) One may generalize the argument in the proofs of propositions I and II in [20] in order to prove that h_j defined by (4.3) are all Lipschitz continuous and hence continuous. However, here in the proof of theorem 11, we used proposition 2.1 established in [19]. (Note that Hurwitz's theorem was used in [19] to prove the continuity of h_j.)

The affirmative solution of problem 3 directly follows from theorem 11. Thus, we have completed the proofs of theorems 4–6, and have attained the goal of the present article.

Here in this article, we have newly established the following eight theorems:

- theorem 4 (practical ALT, $\mathscr{X}_{Hr}(q, 1)$ version),
- theorem 5 (functional ALT, $\mathscr{X}_{Hr}(q, 1)$ version),
- theorem 6 (polynomial ALT, $\mathscr{X}_{Hr}(q, 1)$ version),
- theorem 7 (polynomial closure theorem, $\mathscr{X}_r(q, 1)$-$P(I)$ version),
- theorem 8 (direct sum theorem, $\mathscr{X}_r(q, 1)$ version),
- theorem 9 (functional alpha existence theorem, $\mathscr{X}_{Hr}(q, 1)$-$C(I)$ version),
- theorem 10 (functional alpha representation theorem, $\mathscr{X}_{Hr}(q, 1)$-$C(I)$ version),
- theorem 11 (compatibility theorem, $\mathscr{X}_{Hr}(q, 1)$ version).

In view of the relation (2.6), theorems 1, 4 and 5 in the present article and section 3 of ref. [10], entitled 'The Asymptotic Linearity Theorems that imply the Fukui conjecture,' we now have the following logical implications:

theorem 5 $\Rightarrow$ theorem 4 $\Rightarrow$ theorem 1 $\Rightarrow$ the Fukui conjecture

5. Virtual nanotube tip RST atomic force microscopy and concluding remarks

Carbon nanotubes (CNTs) discovered by Iijima [21] are a new type of carbon fiber made of coaxial cylinders of graphite sheet. This novel material has numerous applications with a direct link to the constantly growing field of nanotechnology [22,23]; an application, for example, is a reusable CNT filter that removes bacterial contaminants like *Escherichia coli* or the nanometer-sized poliovirus from water [24].

With the novel methodology of the RST, one can analyze a sequence of molecular networks, such as a sequence of CNTs, by associating it with a single point of an infinite dimensional vector space: the generalized repeat space

$\mathscr{X}_r(q, 1)$. (This space had been initially defined by the present author in [8] in an axiomatic and general language of $*$-algebras so that the theory can be applied to a variety of molecular problems in a unifying manner.) The RST has provided a totally new way of looking at CNTs. In part I of the present series of articles [9], it has been demonstrated that the RST approach elucidates the conductivity and electron delocalization of CNTs from a novel perspective, and that the RST opens, for the first time, a linkage between (i) the investigative field of CNTs and (ii) that of additivity and reactivity problems of hydrocarbons.

The research program (associated with the present series of articles) entitled *Novel Approach via the Repeat Space Theory to Carbon Nanotubes and Related Molecular Networks*, is directed to cultivate a new interdisciplinary region between the science/technology of CNTs and the modern mathematical theory RST, which now uses the theory of resolution of singularities and algebraic/analytic curves to efficiently analyze the band curves of polymeric materials [19,25]. The guideline of the above research program using the RST, now targeting CNTs under the above-stated title, is the Fukui conjecture (cf. [10] and references therein). The long-range plan of this research program includes investigating this conjecture by developing 'virtual nanotube tip RST atomic force microscopy.' This is a mathematical and computational modeling that simulates a tip of an atomic force microscope modified with a CNT in conjunction with the RST. This modeling provides an ideal system to investigate the asymptotic patterns of structure-property relationships of CNTs, which the Fukui conjecture and related theorems of the RST predict. The software associated with this modeling would be useful not only for scientific investigations of nanotubes but also for educational and pedagogical purposes of training and teaching highly qualified personnel, researchers, and students who are interested in nanoscience and technology.

As mentioned in section 1, we also have hybrid methodology of the repeat space theory and Fukui's reactivity index theory from his frontier orbital theory. This hybrid, which is going to be developed further, can be used for the pattern analysis of functionalization of CNTs. In the initial stage of the above research program, we are going to focus on fundamental research of CNTs and related molecular networks from the novel perspective of the RST. It is within our scope of vision that our new investigative route to nanotubes and related molecular networks will ultimately lead to socially and industrially beneficial applications. Among them are efficient/selective CNT filters that could be produced by controlled functionalization of CNTs and by investigating the surface structure of bundles of CNTs through, e.g., an atomic force microscope and other modern microscopes [26–32].

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