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ORIGINAL PAPER

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

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Abstract The present article is part III of a series devoted to extending the Repeat Space Theory (RST) to apply to carbon nanotubes and related molecular networks. In this part III, four problems concerning the above-mentioned extension of the RST have been formulated. Affirmative solutions of these problems imply (i) asymptotic analysis of carbon nanotubes (CNTs) via the new techniques of normed repeat space, Banach

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.

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algebra, and C^*-algebra becomes possible; (ii) a new linkage is formed between the investigations of CNTs and those of 'spectral symmetry'. In the present paper, we give affirmative solutions to all of the four problems, together with (a) estimates of the norms of matrix sequences representing CNTs, (b) Challenging Problem A$^{\#}$, which complements Problems A, (c) several pictures of 'CNT Matrix Art' which has heuristic power to lead one to get the affirmative answers to the problems formulated in an abstract algebraic manner.

Keywords Repeat space theory (RST) · Carbon nanotubes · *-algebra · Banach algebra · C^*-algebra · Matrix Art

Mathematics Subject Classification 92E10 · 15A18 · 46E15 · 13G05 · 14H20

1 Introduction

The repeat space theory (RST) (cf. [1–24]) is the central unifying theory in the Fukui Project, which was initiated by Kenichi Fukui (1918–1998, Nobel Prize 1981) and has been devoted to cultivating a new interdisciplinary region in science. The reader is referred to [1,2] for the background of the First Generation Fukui Project, and to [2–6] for the development of the Second Generation Fukui Project.

With the novel methodology of the RST, one can analyze a sequence of molecular networks, such as a sequence of single-walled carbon nanotubes (CNTs) (cf. [25–28] and references therein), by associating with it a single element of an infinite dimensional vector space: the generalized repeat space $\mathscr{X}_r(q, d)$, or normed repeat space $\mathscr{X}_r(q, d, p)$ as is shown in the present paper.

These spaces $\mathscr{X}_r(q, d)$ and $\mathscr{X}_r(q, d, p)$ had been initially defined by the first author (S.A.) respectively in ref. [1] and in ref. [3] in an axiomatic and general language of *-algebras, Banach algebra, and C^*-algebras, so that the RST can be applied to a variety of molecular problems in a unifying manner. The space $\mathscr{X}_r(q, d, p)$ is a Banach algebra for all $1 \leq p \leq \infty$, and $\mathscr{X}_r(q, d, p)$ forms a C^*-algebra for $p = 2$. Here, polymer moiety size number q and dimension number d are arbitrarily given positive integers. We remark that the generalized repeat space $\mathscr{X}_r(q, d)$ is contained in the normed repeat space $\mathscr{X}_r(q, d, p)$, which in turn is contained in one of its super spaces $\mathscr{X}_B(q, d, p)$ so that aperiodic polymers can be also represented and investigated in the setting of this super space $\mathscr{X}_B(q, d, p)$. (Cf. [3].)

In this part III, four problems concerning the above-mentioned extension of the RST have been formulated. Affirmative solutions of these problems imply that (i) asymptotic analysis of carbon nanotubes (CNTs) via the new techniques of normed repeat space, Banach algebra, and C^*-algebra becomes possible; (ii) a new linkage is formed between the investigations of CNTs and those of 'spectral symmetry'. In the present paper, we give affirmative solutions to all of the four problems, together with several pictures of 'CNT Matrix Art' which has heuristic power to lead one to get the affirmative answers to the problems formulated in an abstract algebraic manner.

In Sect. 2, after some preparations, we formulate the four problems (Problems A), and solve them in Sect. 3. In Sect. 4, we provide estimates of the norms of matrix sequences representing CNTs and also Challenging Problem A$^{\#}$, which complements Problems A. Section 5 provides pictures from the Matrix Art Program of what is called the Niagra Project, which is a special part of the ongoing international, interdisciplinary, and inter-generational Second Generation Fukui Project.

2 Formulation of Problems A

Before formulating Problems A, we need some preparation.

Throughout, let $\mathbb{Z}^+, \mathbb{Z}_0^+, \mathbb{Z}, \mathbb{R}$, and $\mathbb{C}$, denote respectively the set of all positive integers, nonnegative integers, integers, real numbers, and complex numbers. The reader is asked to briefly read Sect. 2 of the fist part of this series [17] and to recall the following notation.

Matrices $\boldsymbol{L(N, n, t, x, y, z)}$ *and* $\boldsymbol{\tilde{L}(\theta, n, t, x, y, z)}$ Let $r \in \mathbb{Z}^+$, let

$$x, y, z \in \boldsymbol{M}_r(\mathbb{C}) \text{ with } x^* = x. \tag{2.1}$$

Let $N, n \in \mathbb{Z}^+$, and let $t \in \mathbb{Z}$. Define the $rnN \times rnN$ Hermitian matrix $L(N, n, t, x, y, z)$ by

$$\begin{aligned} L(N, n, t, x, y, z) = {} & P_N^{-t} \otimes C_n^* + P_N^{-1} \otimes B_n^* + P_N^0 \otimes \left(A_n - C_n^* - C_n\right) \\ & + P_N^{+1} \otimes B_n + P_N^{+t} \otimes C_n, \end{aligned} \tag{2.2}$$

where

$$A_n = P_n^{-1} \otimes y^* + P_n^0 \otimes x + P_n^{+1} \otimes y, \tag{2.3}$$

$$B_n = P_n^0 \otimes z, \tag{2.4}$$

$$C_n = (P_n S_n) \otimes y. \tag{2.5}$$

Let $\theta \in \mathbb{R}$, define the $rn \times rn$ Hermitian matrix $\tilde{L}(\theta, n, t, x, y, z)$ by

$$\begin{aligned} \tilde{L}(\theta, n, t, x, y, z) = {} & (e^{i\theta})^{-t} C_n^* + (e^{i\theta})^{-1} B_n^* + (e^{i\theta})^0 \left(A_n - C_n^* - C_n\right) \\ & + (e^{i\theta})^{+1} B_n + (e^{i\theta})^{+t} C_n. \end{aligned} \tag{2.6}$$

Matrices $M_N^{n,t,c,d}$ and $F^{n,t,c,d}(\theta)$ defined below (by using the above matrices $L(N, n, t, x, y, z)$ and $\tilde{L}(\theta, n, t, x, y, z)$) play a significant role in the present article.

Matrices $\boldsymbol{M_N^{n,t,c,d}}$ and $\boldsymbol{F^{n,t,c,d}(\theta)}$ Let $N, n \in \mathbb{Z}^+$, and let $t \in \mathbb{Z}$. Let $c, d \in \mathbb{C}$, and let

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y(c) := \begin{pmatrix} 0 & 0 \\ c & 0 \end{pmatrix}, \quad Z(d) := \begin{pmatrix} 0 & 0 \\ d & 0 \end{pmatrix}. \tag{2.7}$$

Define the $2nN \times 2nN$ Hermitian matrix $M_N^{n,t,c,d}$ by

$$M_N^{n,t,c,d} := L\left(N, n, t, X, Y(c), Z(d)\right). \tag{2.8}$$

Let $F^{n,t,c,d} : \mathbb{R} \to \boldsymbol{M}_q(\mathbb{C})$ denote the $2n \times 2n$ Hermitian-matrix-valued function defined by

$$F^{n,t,c,d}(\theta) = \tilde{L}(\theta, n, t, X, Y(c), Z(d)). \tag{2.9}$$

The reader is referred to part I [17] to recall the following Problems (I)–(IV) given in Sect. 6 of part I [17]. Let $a \in \mathbb{Z}^+$, let $b \in \mathbb{Z}$, let $c, d \in \mathbb{C}$, and let $\theta \in \mathbb{R}$.

Problems

(I) Is the sequence $\{M_N^{a,-b,c,d}\}_{N \in \mathbb{Z}^+}$ an element of a generalized repeat space?
(II) Is the sequence $\{F^{n,-b,c,d}(\theta)\}_{n \in \mathbb{Z}^+}$ an element of a generalized repeat space?
(III) Given an $N \in \mathbb{Z}^+$, are all the eigenvalues of the matrix $M_N^{a,-b,c,d}$ explicitly obtainable?
(IV) Given a $\theta \in \mathbb{R}$, are all the eigenvalues of the matrix $F^{a,-b,c,d}(\theta)$ explicitly obtainable?

Our new problems are:

Problems A

(A.1) Is the sequence $\{M_N^{a,-b,c,d}\}_{N \in \mathbb{Z}^+}$ an element of a normed repeat space $\mathscr{X}_r(q, d, p)$?
(A.II) Is the sequence $\{F^{n,-b,c,d}(\theta)\}_{n \in \mathbb{Z}^+}$ an element of a normed repeat space $\mathscr{X}_r(q, d, p)$?
(A.III) Given an $N \in \mathbb{Z}^+$, are all the eigenvalues of the matrix $M_N^{a,-b,c,d}$ explicitly obtainable through the technique of spectral symmetry given in part I of the seven paper series of structural analysis of chemical network systems published in the Int. J. Quantum Chem. [24]?
(A.IV) Given a $\theta \in \mathbb{R}$, are all the eigenvalues of the matrix $F^{a,-b,c,d}(\theta)$ explicitly obtainable through the technique of spectral symmetry given in part I of the seven paper series of structural analysis of chemical network systems published in the Int. J. Quantum Chem. [24]?

We will provide affirmative solutions for the above problems (A.I)–(A.IV) in Sect. 3.

3 Solutions of Problems A

The affirmative solutions of Problems (A.I) and (A.II) can be obtained by recalling Definition 1 of the normed repeat space given in [3]:

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

$$\mathscr{X}_r\left(q, d, p\right) := \text{closure of} \mathscr{X}_r\left(q, d\right) \subset \mathscr{X}_B\left(q, d, p\right). \tag{3.1}$$

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

and by recalling **Theorem 7.1** in part I of this series [17] which asserts that

(I) The sequence $\{M_N^{a,-b,c,d}\}_{N\in\mathbb{Z}^+}$ is an element of $\mathscr{X}_r(2a, 1)$: the generalized repeat space with size $(2a, 1)$.
(II) The sequence $\{F^{n,-b,c,d}(\theta)\}_{n\in\mathbb{Z}^+}$ is an element of $\mathscr{X}_r(2, 1)$: the generalized repeat space with size $(2, 1)$.

Note that an affirmative solution of Problem (A.III) automatically follows from an affirmative solution of Problem (A.IV), since all the eigenvalues of the matrix $M_N^{a,-b,c,d}$ are explicitly obtained by using **Theorem 7.2** in part I of this series [17] and by using the eigenvalues of the matrix $F^{a,-b,c,d}(\theta)$.

Now it remains to give an affirmative solution to Problem (A.IV). To do this, let us at first recall a fundamental tool of spectral symmetry:

Theorem A (Theorem 2 of part I of the Structural Analysis Series from IJQC [24]). *Let E be a finite dimensional linear space over the field $\mathbb{C}$, let $T : E \to E$ be a linear operator, let $\lambda_1, \lambda_2, \ldots, \lambda_r$ be all the distinct eigenvalues of T, let $m(\lambda_i)$ be the algebraic multiplicity of λ_i, and let G_{λ_i} be the generalized eigenspace associated with λ_i, $i \in \{1, 2, \ldots, r\}$. Let ψ be a polynomial with real coefficients, and let $\tau : E \to E$ be a nonsingular (i.e., bijective) linear operator.*

Suppose that

$$\tau^{-1}T\tau = \psi(T). \tag{3.2}$$

Then, the following statements are true:

(i) $\{\lambda_1, \lambda_2, \ldots, \lambda_r\} = \{\psi(\lambda_1), \psi(\lambda_2), \ldots, \psi(\lambda_r)\}$,
(ii) $(m(\lambda_1), m(\lambda_2), \ldots, m(\lambda_r)) = (m(\psi(\lambda_1)), m(\psi(\lambda_2)), \ldots, m(\psi(\lambda_r)))$,
(iii) $(\tau(G_{\lambda_1}), \tau(G_{\lambda_2}), \ldots, \tau(G_{\lambda_r})) = (G_{\psi(\lambda_1)}, G_{\psi(\lambda_2)}, \ldots, G_{\psi(\lambda_r)})$.

To give an affirmative solution of Problem (A.IV), we have only to prove Theorem 7.4 in part I of this series [17] reproduced as Theorem B below by using the above Theorem A. Before reproducing Theorem 7.4, let us recall **Definition 7.1** in part I of this series [17]: For each $n \in \mathbb{Z}^+$, let $\mathrm{Sg}_n : \{1, \ldots, 2n\} \to \{-1, 1\}$ denote the function defined by

$$\mathrm{Sg}_n(j) = \begin{cases} 1 & \text{if} \quad j \in \{1, \ldots, n\}, \\ -1 & \text{if} \quad j \in \{n+1, \ldots, 2n\}. \end{cases} \tag{3.3}$$

Theorem B *Let $n \in \mathbb{Z}^+$, let $t \in \mathbb{Z}$, let $c, d \in \mathbb{C}$, and let $\theta \in \mathbb{R}$. Let*

$$\rho := \rho(d, \theta) = 1 + d^*\exp(-i\theta). \tag{3.4}$$

Then, for $1 \le j \le 2n$, the eigenvalue $\lambda_j^{n,t,c,d}(\theta)$ of the $2n \times 2n$ Hermitian matrix $F^{n,t,c,d}(\theta)$ is given by

$$\lambda_j^{n,t,c,d}(\theta) = \mathrm{Sg}_n(j)\sqrt{|c|^2 + |\rho|^2 + 2\mathrm{Re}\left(c\rho \exp\left(i\left(\frac{t\theta + 2\pi j}{n}\right)\right)\right)} \tag{3.5}$$
$$= \mathrm{Sg}_n(j)\sqrt{|c|^2 + |\rho|^2 + 2\,|c|\,|\rho| \cos\left(\mathrm{Arg}(c) + \mathrm{Arg}(\rho) + \frac{\theta t + 2\pi j}{n}\right)}.$$

Proof Let

$$\varepsilon := \varepsilon(t, \theta) = \exp(it\theta). \tag{3.6}$$

Let $n \in \mathbb{Z}^+$, let $\hat{P}_n$ denote the $n \times n$ unitary matrix defined by $\hat{P}_n = \varepsilon$ if $n = 1$, and

$$\hat{P}_n = \begin{pmatrix} 0 & 1 & & & & & \\ & 0 & 1 & & & \mathbf{0} & \\ & & 0 & \ddots & & & \\ & & & \ddots & \ddots & & \\ & & & & 0 & 1 & \\ & \mathbf{0} & & & & 0 & 1 \\ \varepsilon & & & & & & 0 \end{pmatrix}, \tag{3.7}$$

if $n \ge 2$. Then, the characteristic equation of $\hat{P}_n$ is given by

$$l^n - \varepsilon = 0, \tag{3.8}$$

so that the eigenvalues l_j of $\hat{P}_n$ are given by

$$l_j = \exp\left(i\left(\frac{t\theta + 2\pi j}{n}\right)\right), \tag{3.9}$$

$j \in \{1, \ldots, n\}$. Let

$$\hat{D}_n := \mathrm{diag}(l_1, \ldots, l_n), \tag{3.10}$$

and let $\hat{U}_n$ denote a unitary matrix such that

$$\hat{U}_n^{-1}\hat{P}_n\hat{U}_n = \hat{D}_n. \tag{3.11}$$

We mimic the argument in the proof of theorem 7.2(i) from part I [17], and express the $2n \times 2n$ Hermitian matrix $F^{n,t,c,d}(\theta)$ in terms of c, ρ, and $\hat{P}_n$ as follows:

$$F^{n,t,c,d}(\theta) = \sum_{k=-1}^{1} \hat{P}_n^k \otimes \hat{Q}_k, \tag{3.12}$$

where

$$\hat{Q}_{-1} = \begin{pmatrix} 0 & c^* \\ 0 & 0 \end{pmatrix}, \hat{Q}_0 = \begin{pmatrix} 0 & \rho \\ \rho^* & 0 \end{pmatrix}, \hat{Q}_1 = \begin{pmatrix} 0 & 0 \\ c & 0 \end{pmatrix}. \tag{3.13}$$

Alternatively, we may express the $2n \times 2n$ Hermitian matrix $F^{n,t,c,d}(\theta)$ as follows:

$$F^{n,t,c,d}(\theta) = \begin{pmatrix} 0 & \rho & & & & & & & & c^*\varepsilon^* \\ \rho^* & 0 & c & & & & & & & \\ & c^* & 0 & \rho & & & \mathbf{0} & & & \\ & & \rho^* & 0 & c & & & & & \\ & & & c^* & \bullet & \bullet & & & & \\ & & & & \bullet & \bullet & \bullet & & & \\ & & & & & \bullet & \bullet & \bullet & & \\ & & \mathbf{0} & & & & \bullet & 0 & c & \\ & & & & & & & c^* & 0 & \rho \\ c\varepsilon & & & & & & & & \rho^* & 0 \end{pmatrix}, \tag{3.14}$$

for $n \geq 2$ and

$$F^{n,t,c,d}(\theta) = \begin{pmatrix} 0 & \rho + c^*\varepsilon^* \\ \rho^* + c\varepsilon & 0 \end{pmatrix}, \tag{3.15}$$

for $n = 1$.

Bearing in mind the fact that $|\varepsilon| = 1$, we easily verify that $F^{n,t,c,d}(\theta)$ square has the following form:

$$F^{n,t,c,d}(\theta)^2 = (|c|^2 + |\rho|^2)\hat{P}_{2n}^0 + c\rho\hat{P}_{2n}^2 + c^*\rho^*\hat{P}_{2n}^{-2}. \tag{3.16}$$

Note that the eigenvalues μ_j of $\hat{P}_{2n}$ are given by

$$\mu_j = \exp\left(i\left(\frac{t\theta + 2\pi j}{2n}\right)\right), \tag{3.17}$$

$j \in \{1, \ldots, 2n\}$ and that the eigenvalues ξ_j of $F^{n,t,c,d}(\theta)^2$ are given by

$$\xi_j = |c|^2 + |\rho|^2 + c\rho\mu_j^2 + c^*\rho^*\mu_j^{-2}, \tag{3.18}$$

$j \in \{1, \ldots, 2n\}$. Since $\mu_j = \mu_{n+j}$ for all $j \in \{1, \ldots, n\}$, we have

$$\xi_j = \xi_{n+j} \tag{3.19}$$

for all $j \in \{1, \ldots, n\}$.

Let $\omega = -1$ and let

$$\tau := \mathrm{diag}(\omega^1, \omega^2, \ldots, \omega^{2n}), \tag{3.20}$$

then we have

$$\begin{aligned}\left(\tau^{-1} F^{n,t,c,d}(\theta)\tau\right)_{ij} &= \omega^{-i+j}\left(F^{n,t,c,d}(\theta)\right)_{ij} \\ &= (-1)^{-i+j}\left(F^{n,t,c,d}(\theta)\right)_{ij}.\end{aligned} \tag{3.21}$$

By noticing the fact that $(F^{n,t,c,d}(\theta))_{ij}$ vanishes whenever $-i + j$ is an even number, we see that

$$\left(\tau^{-1} F^{n,t,c,d}(\theta)\tau\right)_{ij} = (-1)\left(F^{n,t,c,d}(\theta)\right)_{ij}, \tag{3.22}$$

for all $i, j \in \{1, 2, \ldots, 2n\}$, thus we have

$$\tau^{-1} F^{n,t,c,d}(\theta)\tau = (-1)\, F^{n,t,c,d}(\theta). \tag{3.23}$$

Before applying Theorem A, it is convenient at this moment to introduce

Lemma 1 *Let $\xi_1, \xi_2, \ldots, \xi_n$ be nonnegative real numbers. Let F be a $2n \times 2n$ Hermitian matrix, let $\sigma(F)$ denote the spectrum of F (the set of all eigenvalues of F). Let $m(\lambda)$ denote the algebraic multiplicity of $\lambda \in \sigma(F)$. Suppose that the following conditions (i) and (ii) hold:*

(i) *For each $\lambda \in \sigma(F)$,*

$$-\lambda \in \sigma(F), \tag{3.24}$$
$$m(-\lambda) = m(\lambda). \tag{3.25}$$

(ii) *There exists a $2n \times 2n$ unitary matrix V such that*

$$V^{-1} F^2 V = \mathrm{diag}(\xi_1, \xi_2, \ldots, \xi_n, \xi_1, \xi_2, \ldots, \xi_n). \tag{3.26}$$

Then, we have

(iii) *There exists a $2n \times 2n$ unitary matrix W such that*

$$W^{-1} F W = \mathrm{diag}\left(\sqrt{\xi_1}, \sqrt{\xi_2}, \ldots, \sqrt{\xi_n}, -\sqrt{\xi_1}, -\sqrt{\xi_2}, \ldots, -\sqrt{\xi_n}\right). \tag{3.27}$$

Proof of Lemma 1 Assume (i) and (ii). Let $\lambda_j(F)$ denote the jth eigenvalue of F counted with multiplicity, arranged in the increasing order, where $j \in \{1, \ldots, n\}$.

Then, (i) implies that

$$\lambda_1(F) \leq \lambda_2(F) \leq \cdots \leq \lambda_{2n}(F), \tag{3.28}$$

and that

$$-\lambda_j(F) = \lambda_{2n+1-j}(F) \tag{3.29}$$

for all $j \in \{1, \ldots, n\}$. Thus, there exist n nonnegative real numbers

$$0 \leq \varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_n \tag{3.30}$$

and a $2n \times 2n$ unitary matrix U such that

$$U^{-1} F U = \mathrm{diag}(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n, -\varepsilon_1, -\varepsilon_2, \ldots, -\varepsilon_n). \tag{3.31}$$

Squaring both sides, we have

$$U^{-1} F^2 U = \mathrm{diag}(\varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2, \varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2). \tag{3.32}$$

Now compare (3.26) with (3.32) and note that $\xi_1, \xi_2, \ldots, \xi_n, \xi_1, \xi_2, \ldots, \xi_n$ and $\varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2, \varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2$ are both $2n$ eigenvalues of F^2. From this fact we easily infer that there is a bijection (permutation) $s : \{1, \ldots, n\} \to \{1, \ldots, n\}$ and a $2n \times 2n$ permutation (unitary) matrix P such that

$$\begin{aligned} &\mathrm{diag}\left(\varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2, \varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2\right) \\ &= \mathrm{diag}\left(\xi_{s(1)}, \xi_{s(2)}, \ldots, \xi_{s(n)}, \xi_{s(1)}, \xi_{s(2)}, \ldots, \xi_{s(n)}\right) \\ &= P \mathrm{diag}\left(\xi_1, \xi_2, \ldots, \xi_n, \xi_1, \xi_2, \ldots, \xi_n\right) P^{-1}. \end{aligned} \tag{3.33}$$

(**Note**: Let $\alpha_1 < \alpha_2 < \cdots < \alpha_r$ be r nonnegative real numbers such that $\sigma(F^2) = \{\alpha_1, \alpha_2, \ldots, \alpha_r\}$, where $r \leq n$. To construct a permutation s on $\{1, \ldots, n\}$ that satisfies the first equality of (3.33), select a permutation s so that $\xi_{s(1)} \leq \xi_{s(2)} \leq \cdots \leq \xi_{s(n)}$. Let $E := (\varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2)$ and let $X := (\xi_{s(1)}, \xi_{s(2)}, \ldots, \xi_{s(n)})$ and express E and X in terms of α_j:

$$E = (\alpha_1, \ldots, \alpha_1, \alpha_2, \ldots, \alpha_2, \ldots, \alpha_r, \ldots \alpha_r), \tag{3.34}$$

where each α_j is repeated k_j times,

$$X = (\alpha_1, \ldots, \alpha_1, \alpha_2, \ldots, \alpha_2, \ldots, \alpha_r, \ldots \alpha_r), \tag{3.35}$$

where each α_j is repeated l_j times. By the fact that $\xi_1, \xi_2, \ldots, \xi_n, \xi_1, \xi_2, \ldots, \xi_n$ and $\varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2, \varepsilon_1^2, \varepsilon_2^2, \ldots, \varepsilon_n^2$ are both $2n$ eigenvalues of F^2, we see that

$$m(\alpha_j) = 2k_j = 2l_j \tag{3.36}$$

for all $j \in \{1, \ldots, r\}$. Thus, we have

$$E = X, \tag{3.37}$$

constructing a permutation s that satisfies the first equality of (3.33).)

On the other hand, since ε_j are all nonnegative, we see that

$$\varepsilon_j = \sqrt{\xi_{s(j)}} \tag{3.38}$$

for all $j \in \{1, \ldots, n\}$. Thus, making the substitution (3.38) in (3.31), we obtain:

$$\begin{aligned} U^{-1}FU &= \mathrm{diag}\left(\sqrt{\xi_{s(1)}}, \sqrt{\xi_{s(2)}}, \ldots, \sqrt{\xi_{s(n)}}, -\sqrt{\xi_{s(1)}}, -\sqrt{\xi_{s(2)}}, \ldots, -\sqrt{\xi_{s(n)}}\right) \\ &= P\mathrm{diag}\left(\sqrt{\xi_1}, \sqrt{\xi_2}, \ldots, \sqrt{\xi_n}, -\sqrt{\xi_1}, -\sqrt{\xi_2}, \ldots, -\sqrt{\xi_n}\right) P^{-1}. \end{aligned} \tag{3.39}$$

Therefore, we see that

$$P^{-1}U^{-1}FUP = \mathrm{diag}\left(\sqrt{\xi_1}, \sqrt{\xi_2}, \ldots, \sqrt{\xi_n}, -\sqrt{\xi_1}, -\sqrt{\xi_2}, \ldots, -\sqrt{\xi_n}\right). \tag{3.40}$$

By setting

$$W = UP, \tag{3.41}$$

since $W^{-1} = P^{-1}U^{-1}$, we get (iii). □

Now apply Theorem A and notice that the spectrum of $F^{n,t,c,d}(\theta)$ has the (-1)-rotational symmetry counting the multiplicity. Recall Eq. (3.19) and compare it with condition (ii) of Lemma 1.

By Lemma 1, we see that the eigenvalues of $F^{n,t,c,d}(\theta)$ are given by

$$\begin{aligned} &\pm\sqrt{|c|^2 + |\rho|^2 + c\rho\mu_j^2 + c^*\rho^*\mu_j^{-2}} \\ &= \pm\sqrt{|c|^2 + |\rho|^2 + 2\mathrm{Re}[c\rho\mu_j^2]} \\ &= \pm\sqrt{|c|^2 + |\rho|^2 + 2\mathrm{Re}\left(c\rho\exp\left(i\left(\frac{t\theta + 2\pi j}{n}\right)\right)\right)}, \end{aligned} \tag{3.42}$$

$j \in \{1, \ldots, n\}$. From this the conclusion follows. □

Now all of our Problems (A.I)–(A.IV) have been affirmatively solved. Thus, we have established theoretical linkages between the present series of articles and the following:

(i) Part I of the structural analysis series [17] and related investigations (cf. [14] and references therein),
(ii) Theorm I in ref. [4] entitled 'Fundamental notions for the second generation Fukui project and a prototypal problem of the normed repeat space and its super spaces', so that asymptotic analysis of sequences of CNTs is possible by using Theorem I in [4] and related notions of Banach algebras and C^*-algebras.
(iii) Challenging Parallel Problems II, III, and IV [4], which are directly related to the problems of 'spectral symmetry'.

4 Estimates of the norms of matrix sequences representing CNTs and Challenging Problem A#

(I) The sequence $\{M_N^{a,-b,c,d}\}_{N\in\mathbb{Z}^+}$ is an element of $\mathscr{X}_B(2a,1,2)$.
(II) The sequence $\{F^{n,-b,c,d}(\theta)\}_{n\in\mathbb{Z}^+}$ is an element of $\mathscr{X}_B(2,1,2)$.

The above propositions (I) and (II) can be directly established by proving the following and similar estimates:

$$\sup_{N\geq 1}\left\| M_N^{a,-b,c,d}\right\|_2 \leq |c|+|d|+1<\infty, \tag{4.1}$$

$$\sup_{n\geq 1}\left\| F^{n,-b,c,d}(\theta)\right\|_2 \leq |c|+|d|+1<\infty. \tag{4.2}$$

From the explicitly obtained eigenvalues (3.5), one can get the following estimate of the norm of Hermitian matrix $F^{n,-b,c,d}(\theta)$:

$$\begin{aligned}
\left\| F^{n,-b,c,d}(\theta)\right\|_2 &= \max_j \left|\lambda_j(F^{n,-b,c,d}(\theta)^2)\right|^{\frac{1}{2}} \\
&= \max_j \left||c|^2+|\rho|^2+c\rho\mu_j^2+c^*\rho^*\mu_j^{-2}\right|^{\frac{1}{2}} \\
&= \max_j \left||c|^2+\left|1+d^*e^{-i\theta}\right|^2+c(1+d^*e^{-i\theta})\mu_j^2+c^*(1+de^{i\theta})\mu_j^{-2}\right|^{\frac{1}{2}} \\
&\leq \left(|c|^2+(1+|d|)^2+2\,|c|\,(1+|d|)\right)^{\frac{1}{2}} \\
&= |c|+|d|+1.
\end{aligned} \tag{4.3}$$

For carbon nanotubes, setting $c=d=1$, we see that the above upper bound agrees with the maximal vertex degree in the nanotube graphs, which is 3. See also the Matrix Art pictures of CNT energy band curves given in Figs. 3 and 4 in Sect. 5 and note that $|Energy|\leq 3$ in the pictures.

Now we are ready to formulate our

Challenging Problem A# Is it possible to get the above and similar estimates of norms without using the explicitly obtained eigenvalues of $F^{n,-b,c,d}(\theta)$?

This problem complements our Problem A formulated in Sect. 2. The study of this and associated challenging problems enriches the interdisciplinary investigation

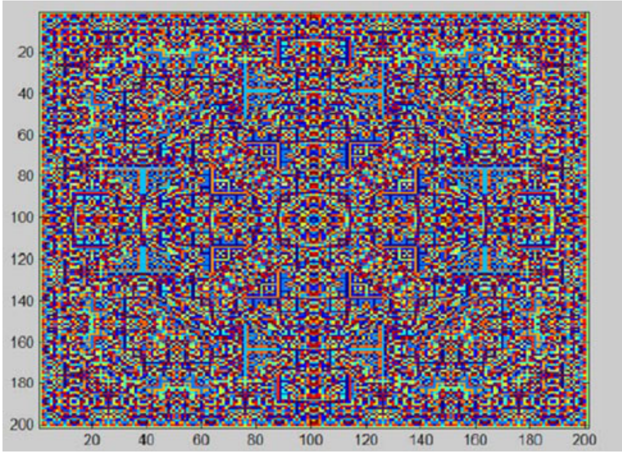

Fig. 1 Matrix Art picture called 'Carpet 1'

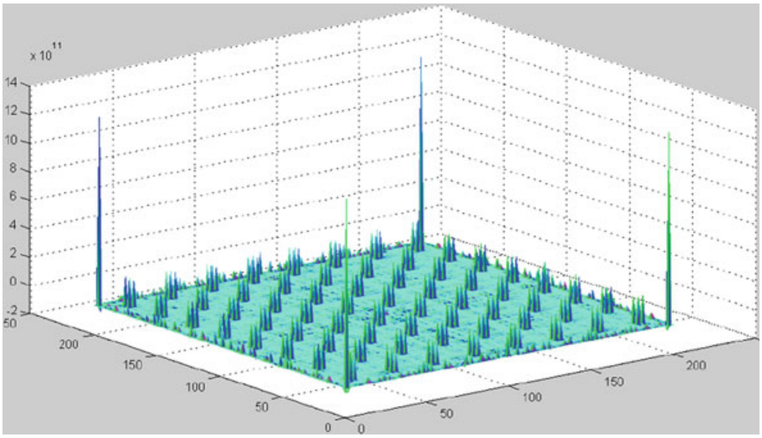

Fig. 2 Matrix Art picture called 'Bamboos'

related to carbon nanotubes and other molecular networks. The affirmative solutions for the above Challenging Problem $A^{\#}$ and related problems will be published elsewhere.

5 Matrix Art of CNT energy band curves and energy surfaces

In a recent article [6] by the first author (S.A.), various pictures of Matrix Art of 'Magic Mountains' having inwardly repeating fractal structures were provided. Cf. article [6] for our motivation of investigating inwardly repeating fractal structures (cf. also [23,29,30] and references therein) for the study of molecular networks having many identical moieties. The reader is referred to [4,6] and references therein for the origin of Matrix Art. The Matrix Art pictures in Figs. 1 and 2 given above are

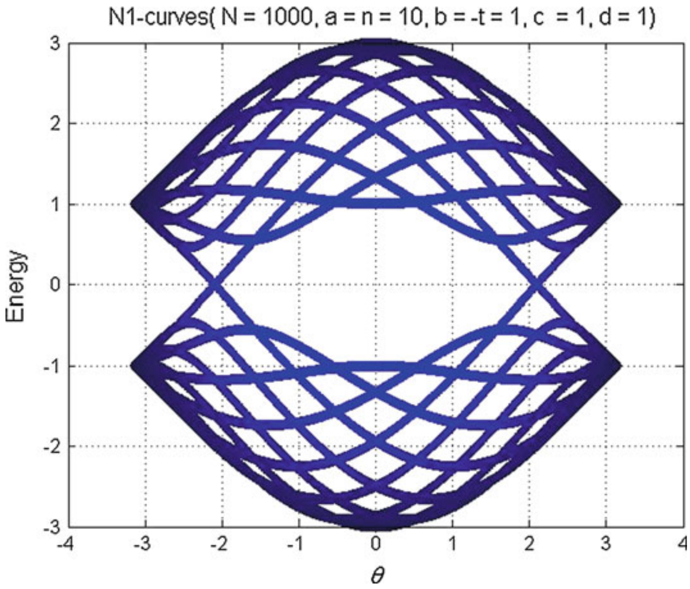

Fig. 3 Matrix Art picture of CNT energy band curves called 'Cradles'

respectively called 'Carpet 1' and 'Bamboos'. These were created in the Matrix Art Challenge Seminar in Tsuyama National College of Technology by using MagicMt$_0$ defined in [6].

In what follows, we present pictures of Matrix Art of CNT energy band curves and CNT energy band surfaces, which were created in the Matrix Art Challenge Seminar in Tsuyama National College of Technology. We remark that symmetry found in those pictures in Figs. 3, 4, 5, 6, 7 and 8 played a heuristic role motivating us to provide an affirmative solution of our Problem (A.IV) formulated in Sect. 2 of the present article.

The reader is also invited to refer to Prof. H. Hironaka's public speech entitled 'Mathematics and the Sciences' [31] for an instructive account of the notion of self-similarity, fractal geometry, and of mathematical sciences.

The reader is also invited to refer to Prof. R. Hoffmann's public speech entitled 'One Culture' [32]. We would like to record here the fact that two refs. [31,32] formed an important source of inspiration for the Fukui Project, which is devoted to cultivating a new interdisciplinary region in science, often utilizing dialectic interplay between a complementary pair of opposite notions and ideas. These two refs. [31,32] are also playing a role of a guideline for the Matrix Art Program of what is called the Niagara Project (cf. [4,6,11] for details), which is a special new part of the on-going international, interdisciplinary, and inter-generational Second Generation Fukui Project.

In ref. [11], entitled 'Proof of the Fukui conjecture via resolution of singularities and related methods. V', theory of analytic (highly smooth) curves and resolution of singularities has been applied to prove the Fukui conjecture originating in chemistry.

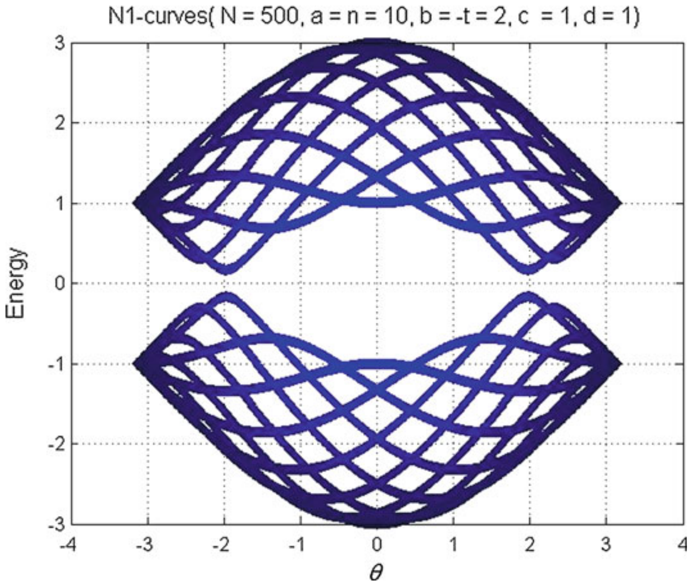

Fig. 4 Matrix Art picture of CNT energy band curves called 'Baskets'

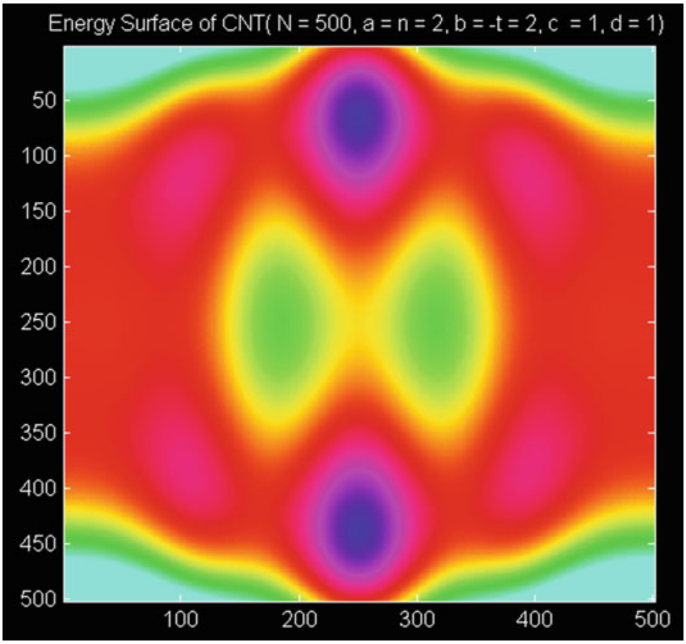

Fig. 5 Matrix Art picture of CNT energy band surface called 'Face 1'

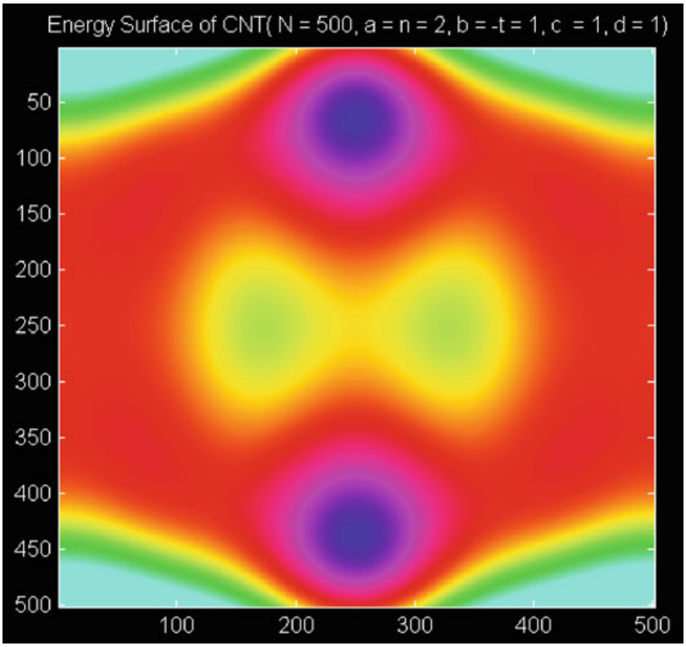

Fig. 6 Matrix Art picture of CNT energy band surfaces called 'Face 2'

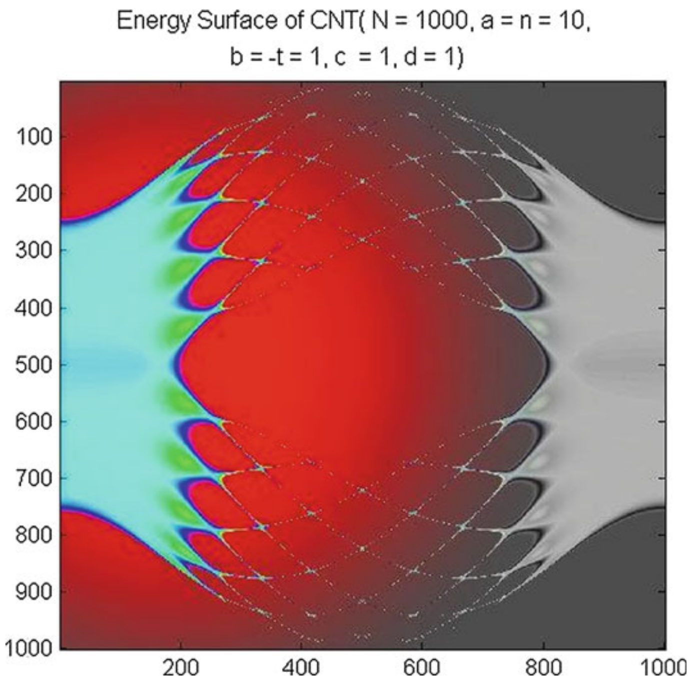

Fig. 7 Matrix Art picture of CNT energy band surfaces called 'Cat's Cradle 1'

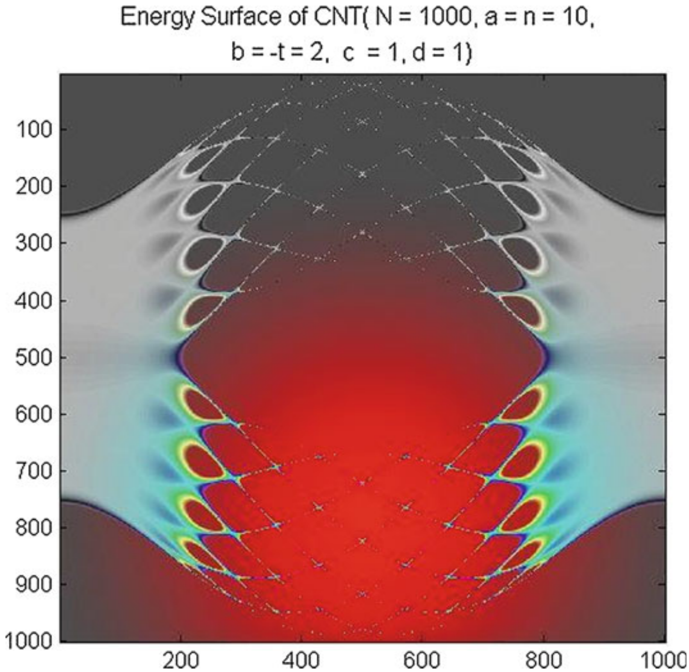

Fig. 8 Matrix Art picture of CNT energy band surfaces called 'Cat's Cradle 2'

We remark that

1. the present 'CNT Series' of articles is closely associated with the above-mentioned 'Resolution of Singularities Series I–V' published in the JOMC (cf. ref [11] and references therein for details);
2. the investigations of highly smooth functions and of highly irregular functions are complementary in the repeat space theory (RST), which is the central unifying theory in the Second Generation Fukui Project.

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