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

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The present article is the first part of a series devoted to extending the Repeat Space Theory (RST) to apply to carbon nanotubes and related molecular networks. Four key problems are formulated whose affirmative solutions imply the formation of the initial investigative bridge between the research field of nanotubes and that of the additivity and other network problems studied and solved by using the RST. All of these four problems are solved affirmatively by using tools from the RST. The Piecewise Monotone Lemmas (PMLs) are cornerstones of the proof of the Fukui conjecture concerning the additivity problems of hydrocarbons. The solution of the fourth problem gives a generalized analytical formula of the pi-electron energy band curves of nanotube (a, b), with two new complex parameters c and d. These two parameters bring forth a broad class of analytic curves to which the PMLs and associated theoretical devices apply. Based on the above affirmative solutions of the problems, a central theorem in the RST, called the asymptotic linearity theorem (ALT) has been applied to nanotubes and monocyclic polyenes. Analytical formulae derived in this application of the ALT illuminate in a new global context (i) the conductivity of nanotubes and (ii) the aromaticity of monocyclic polyenes; moreover an analytical formula obtained by using the ALT provides a fresh insight into Hückel's $(4n + 2)$ rule. The present article forms a foundation of the forthcoming articles in this series.

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

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1. Introduction

The repeat space theory (RST) originated in the empirical analysis of thermodynamic and spectroscopic data on organic compounds. It initially concerned

*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.

the correlation between structure and properties in molecules having many identical moieties. In recent years, interacting with the theories of dynamical systems, operator algebra, and so forth, the RST has developed into a comprehensive theoretical framework of axiomatic nature (cf. [1–8]), which unites and solves a variety of problems, in particular, of physicochemical networks in a new global context.

By using a theoretical device from the RST, it can be demonstrated [9] that the formula of the pi-electron energy band curves of carbon nanotubes expounded in ref. [10] provides strikingly ample examples of the analytic curves to which the Piecewise Monotone Lemmas (PMLs) can be applied. The PMLs are cornerstones of the proof of the Fukui conjecture (concerning the additivity problems of hydrocarbons) which continues to be of vital significance in the new development of the generalized repeat space, and also in view of the new applications of resolution of singularities and the theory of algebraic and analytic curves to physicochemical networks. (This conjecture was proved by the present author [11–13] and has been further investigated in the series of papers entitled 'Proof of the Fukui conjecture via resolution of singularities and related methods' [14,15].)

The single-wall nanotubes treated in ref. [10] can be regarded as fused benzene molecular networks in the form of cylinder. (Cf. [10,16,17] and references therein, and cf. section 3 of the present paper for the representation of nanotubes using abelian groups. Cf. also remarks 7.1 in section 7 on a comparative study of toroidal carbon nanotubes and their linear counterparts.) Since the additivity and other network problems of conjugated molecular networks including fused benzenes have been well studied by means of the RST, it is natural to ask if the RST is applicable to the research of carbon nanotubes and conversely if the latter can enhance the development of the RST, which now uses the theory of algebraic and analytic curves, and resolution of singularities.

After several steps of preparations, we formulate four key problems in section 6. The first two problems concern the question of whether or not the eigenvalue problem associated with nanotube(a, b) treated in ref. [10] can be stated in the operator-theoretic setting of the RST, namely within the structure of the $*$-algebra of the repeat space $\mathscr{X}_r(q, 1)$. The last two problems deal with the question of whether it is possible to obtain a generalized analytic formula of the pi-electron energy band curves of nanotube(a, b), with two new complex parameters c and d. These two parameters bring forth a broader set of analytic curves to which the PMLs and the associated theoretical devices are applicable.

All of these four problems are affirmatively answered in section 7. These solutions pave, for the first time, the investigative connection between the research field of nanotubes and that of the additivity and other network problems studied and solved by using the RST.

The crucial tools from the RST for the solutions of the key problems are:

(I) the notion called the standard alpha space with size $(q, 1)$, denoted by $\mathscr{X}_{\#\alpha}(q, 1)$,

(II) the notion of a hyper-circulant, which is a far reaching generalization of a circulant (cf. section 4), and its associated technique called the plug-in block-diagonalization method, or the PB method for short.

Besides being able to indicate *how* to obtain the desired analytical formulae of the general energy band curves, these and related tools from the RST can lead one to get an insight, in a global context, into the reason *why* they are obtainable. Moreover, this insight naturally leads one to notice that in the repeat space $\mathscr{X}_r(q, d)$ with any positive block-size number q and any positive dimension number d, there exists a broad class of analytically diagonalizable matrix sequences that had been hitherto unknown.

In the RST, the asymptotic linearity theorems (ALTs) play a central role in tackling a variety of additivity problems. In sections 8 and 9, based on the above mentioned affirmative solutions of the problems, the functional version of the ALT, which was proved in [2], has been applied for the first time to nanotubes and monocyclic polyenes. Analytical formulae derived in this application of the ALT illuminate in a global context (i) the conductivity of nanotubes and (ii) the aromaticity of monocyclic polyenes; moreover proposition 9.1 in section 9, using the ALT, provides a fresh insight into Hückel's $(4n + 2)$ rule.

The new analytical formulae together with other theoretical tools and techniques developed in the present article form a foundation for the forthcoming parts of this series of articles, which is closely associated with the above mentioned series of articles [14,15] concerning the proof of the Fukui conjecture via resolution of singularities.

We shall start the next section with introducing the basic symbols used in the present article.

2. Definitions of symbols

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. For each positive integer n, $\boldsymbol{M}_n(\mathbb{C})$ denotes the set of all $n \times n$ complex matrices.

Let Arg: $\mathbb{C} \to]-\pi, \pi]$ denote the function defined by

$$\operatorname{Arg}(z) = \begin{cases} 0 & \text{if } z = 0 \\ \theta & \text{if } z \in \mathbb{C} - \{0\}, \end{cases} \tag{2.1}$$

where $\theta \in]-\pi, \pi]$ and

$$z = |z| \exp(i\theta). \tag{2.2}$$

(Note that for each $z \in \mathbb{C} - \{0\}$, there is a unique $\theta \in]-\pi, \pi]$ such that (2.2) holds.)

If S_1 and S_2 are subsets of $\mathbb{C}$ and $z \in \mathbb{C}$, let

$$S_1 + S_2 := \{r_1 + r_2 : r_1 \in S_1, r_2 \in S_2\}, \tag{2.3}$$

$$zS_1 := \{zr_1 : r_1 \in S_1\}. \tag{2.4}$$

By 'for all $N \gg 0$', we mean 'for all positive integers N greater than some given positive integer'. Suppose that Prp(1), Prp(2), ... is an infinite sequence of propositions, then 'Prp(N) is true for all $N \gg 0$' if and only if there exists a positive integer N_0 such that Prp(N) is true for all N greater than N_0. The phrase 'for all $N \gg 0$' conventionally reads 'for all large enough N's'.

Let I_N denote the $N \times N$ identity matrix. If M is an $N \times N$ complex matrix, M^0 denotes the $N \times N$ identity matrix I_N, M^T denotes the transposed matrix of M, and M^* denotes the adjoint matrix of M.

In what follows, we recall the definitions of matrices P_N and S_N which played a fundamental role in constructing the notion of the generalized repeat space (cf. ref. [4] and the appendix). The matrices P_N and S_N and related notions are significant in investigating carbon nanotubes via the RST. From this theory, we shall selectively recall only essential tools necessary for the purpose of this paper.

For each $N \in \mathbb{Z}^+$, P_N denotes an $N \times N$ real-orthogonal matrix given by

$$P_N = \begin{pmatrix} 0 & 1 & & & & & \\ & 0 & 1 & & & \mathbf{0} & \\ & & 0 & \ddots & & & \\ & & & \ddots & \ddots & & \\ & & & & 0 & 1 & \\ & \mathbf{0} & & & & 0 & 1 \\ 1 & & & & & & 0 \end{pmatrix}. \tag{2.5}$$

In other words, P_N is the $N \times N$ cyclic shift matrix with $(P_N)_{ij} = 1$ if $j - i \equiv 1 \mod N$; $(P_N)_{ij} = 0$ otherwise.

For each $N \in \mathbb{Z}^+$, with $j \in \{-2, -3, \ldots\}$ is defined to be $(P_N^{-1})^{-j}$, which equals the transpose of P_N^{-j}. Note that for each $N \in \mathbb{Z}^+$, $j, k \in \mathbb{Z}$, we have

$$P_N^j P_N^k = P_N^{j+k}, \tag{2.6}$$

$$P_N^N = P_N^0, \tag{2.7}$$

$$P_N^{N-j} = P_N^{-j}. \tag{2.8}$$

For each $N \in \mathbb{Z}^+$, let S_N denote an $N \times N$ real matrix given by

$$S_N = \begin{pmatrix} 1 & 0 & & & & & \\ 0 & 0 & 0 & & & \mathbf{0} & \\ & 0 & 0 & \ddots & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & 0 & 0 & \\ & \mathbf{0} & & & 0 & 0 & 0 \\ & & & & & 0 & 0 \end{pmatrix}. \tag{2.9}$$

In other words, S_N is the $N \times N$ matrix defined by $(S_N)_{ij} = 1$ if $i = j = 1$; $(S_N)_{ij} = 0$ otherwise. Note that $(P_N S_N)_{ij} = 1$ if $i = N$ and $j = 1$; $(P_N S_N)_{ij} = 0$ otherwise.

If A is an $m \times m$ complex matrix and B is an $n \times n$ complex matrix, the Kronecker product of the two matrices, denoted by $A \otimes B$ is defined as the partitioned matrix

$$A \otimes B := \begin{pmatrix} A_{11}B & A_{12}B & \cdots & \cdots & A_{1m}B \\ A_{21}B & A_{22}B & \cdots & \cdots & A_{2m}B \\ \vdots & \vdots & & & \vdots \\ \vdots & \vdots & & & \vdots \\ A_{m1}B & A_{m2}B & \cdots & \cdots & A_{mm}B \end{pmatrix}. \tag{2.10}$$

$A \otimes B$ is a matrix of order $(mn \times mn)$. It has m^2 blocks, the (i, j)th block is the matrix $A_{ij}B$ of order $(n \times n)$, thus it is often signified as $A \otimes B = [A_{ij}B]$. The following fundamental formulae for the Kronecker product are easily verifiable (cf. e.g., [18,19]).

$$(A \otimes B) \otimes C = A \otimes (B \otimes C), \tag{2.11}$$
$$(kA) \otimes B = A \otimes (kB) = k(A \otimes B), \quad k \in \mathbb{C}, \tag{2.12}$$
$$A \otimes (B + C) = A \otimes B + A \otimes C, \tag{2.13}$$
$$(A + B) \otimes C = A \otimes C + B \otimes C, \tag{2.14}$$
$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD), \tag{2.15}$$
$$(A \otimes B)^T = A^T \otimes B^T, \tag{2.16}$$
$$(A \otimes B)^* = A^* \otimes B^*, \tag{2.17}$$

where the orders of the matrices involved are such that all the operations are well-defined.

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

$$x, y, z \in \boldsymbol{M}_r(\mathbb{C}) \text{ with } x^* = x. \tag{2.18}$$

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

$$L(N,n,t,x,y,z) = P_N^{-t} \otimes C_n^* + P_N^{-1} \otimes B_n^* + P_N^0 \otimes (A_n - C_n^* - C_n) + P_N^{+1} \otimes B_n + P_N^{+t} \otimes C_n, \tag{2.19}$$

where

$$A_n = P_n^{-1} \otimes y^* + P_n^0 \otimes x + P_n^{+1} \otimes y, \tag{2.20}$$

$$B_n = P_n^0 \otimes z, \tag{2.21}$$

$$C_n = (P_n S_n) \otimes y. \tag{2.22}$$

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

$$\tilde{L}(\theta,n,t,x,y,z) = (e^{i\theta})^{-t} C_n^* + (e^{i\theta})^{-1} B_n^* + (e^{i\theta})^0 (A_n - C_n^* - C_n) + (e^{i\theta})^{+1} B_n + (e^{i\theta})^{+t} C_n. \tag{2.23}$$

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, they are going to be used in the formulation of problems in section 6.

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

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y(c) := \begin{pmatrix} 0 & 0 \\ c & 0 \end{pmatrix}, \quad Z(d) := \begin{pmatrix} 0 & 0 \\ d & 0 \end{pmatrix}. \tag{2.24}$$

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

$$M_N^{n,t,c,d} := L(N, n, t, X, Y(c), Z(d)). \tag{2.25}$$

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

$$F^{n,t,c,d}(\theta) = \tilde{L}(\theta, n, t, X, Y(c), Z(d)). \tag{2.26}$$

3. Representation of nanotube(a, b) using abelian groups

There are several distinct ways of representing nanotube(a, b). We establish here the method of using the complex plane, to which the hexagonal lattice – the pattern of the graphite sheet, is associated, rotated, cut, and glued by means of group theoretical techniques.

In the complex plane $\mathbb{C}$, consider the regular hexagon with edges of the unit length whose vertices are given by

$$z_j = \exp(i(\pi/2 + (j-1)\pi/3)), \tag{3.1}$$

where $j = 1, \ldots, 6$. Let $\mathrm{Ed}(z_j, z_{j+1})$ denote the edge from vertex z_j to vertex z_{j+1}:

$$\mathrm{Ed}(z_j, z_{j+1}) = \{(1-t)z_j + tz_{j+1} : 0 \leqslant t \leqslant 1\}, \tag{3.2}$$

and let $\mathrm{Ed}_0(z_j, z_{j+1})$ denote the edge from vertex z_j to vertex z_{j+1} with both ends excluded:

$$\mathrm{Ed}_0(z_j, z_{j+1}) = \{(1-t)z_j + tz_{j+1} : 0 < t < 1\}, \tag{3.3}$$

where $j = 1, \ldots, 6$, and $z_7 = z_1$.

Let

$$u := z_6 - z_4 = \sqrt{3}/2 + 3i/2, \tag{3.4}$$

$$v := z_2 - z_4 = -\sqrt{3}/2 + 3i/2. \tag{3.5}$$

Put

$$G = \mathbb{C}, \tag{3.6}$$

and note that G forms an abelian group with the addition operation.

For $a \in \mathbb{Z}^+$, $b \in \mathbb{Z}$, $N \in \mathbb{Z}^+ \cup \{\infty\}$, let

$$H_N^{a,b} := \begin{cases} (au + bv)\mathbb{Z} + (0u + Nv)\mathbb{Z} & \text{if } N \in \mathbb{Z}^+, \\ (au + bv)\mathbb{Z} + (0u + 0v)\mathbb{Z} & \text{if } N = \infty, \end{cases} \tag{3.7}$$

and let

$$H_0 := H_1^{1,0} = u\mathbb{Z} + v\mathbb{Z}. \tag{3.8}$$

Notice that the subset $p_1\mathbb{Z} + p_2\mathbb{Z}$ forms a subgroup of G whenever p_1 and p_2 are in G. In fact, $p_1\mathbb{Z} + p_2\mathbb{Z}$ is the smallest subgroup that contains $\{p_1, p_2\} \subset G$, in other words, $p_1\mathbb{Z} + p_2\mathbb{Z}$ is the subgroup of G generated by its subset $\{p_1, p_2\}$. Thus, $H_N^{a,b}$ is a subgroup of the abelian group G.

For each $p \in G$, let $T_p : G \to G$ denote the translation function defined by

$$T_p(z) = z + p. \tag{3.9}$$

Let T_G denote the abelian group of all the translations in G

$$T_G = \{T_p : p \in G\}. \tag{3.10}$$

If G_0 is a subgroup of G, T_{G_0} denotes the subgroup of T_G defined by

$$T_{G_0} := \{T_p : p \in G_0\}. \tag{3.11}$$

Note that T_{H_0} is a subgroup of T_G generated by the subset $\{T_u, T_v\}$.

Let 2^G denote the set of all subsets of G, and let Hex: $\mathbb{Z} \times \mathbb{Z} \to 2^G$ denote the mapping defined by

$$\mathrm{Hex}(\xi_1, \xi_2) := \bigcup_{j=1}^{6} \mathrm{Ed}(z_j, z_{j+1}) + \{u\xi_1 + v\xi_2\}. \tag{3.12}$$

Then the range $\mathrm{Hex}(\mathbb{Z} \times \mathbb{Z})$ of this mapping satisfies the following relation

$$\mathrm{Hex}(\mathbb{Z} \times \mathbb{Z}) = \mathrm{Hex}(0, 0) + H_0, \tag{3.13}$$

it represents the hexagonal lattice in G that contains the set Hex(0, 0) and is invariant under the translations of group T_{H_0}. Note that each hexagon in the hexagonal lattice $\mathrm{Hex}(\mathbb{Z} \times \mathbb{Z})$ is associated to the ordered pair $(\xi_1, \xi_2) \in \mathbb{Z} \times \mathbb{Z}$.

Let

$$E_1 := \mathrm{Ed}_0(z_1, z_2) + H_0, \tag{3.14}$$
$$E_2 := \mathrm{Ed}_0(z_2, z_3) + H_0, \tag{3.15}$$
$$E_3 := \mathrm{Ed}_0(z_3, z_4) + H_0, \tag{3.16}$$
$$E_4 := G - (E_1 \cup E_2 \cup E_3). \tag{3.17}$$

It is easily seen that the sets E_1, E_2, E_3, and E_4 are pairwise disjoint and that they are all invariant under the translations of group T_{H_0}.

Let $c, d \in \mathbb{R}$, and let $f^{c,d} : G \to \mathbb{R}$ be the function defined by

$$f^{c,d}(z) = \begin{cases} c & \text{if } z \in E_1, \\ 1 & \text{if } z \in E_2, \\ d & \text{if } z \in E_3, \\ 0 & \text{if } z \in E_4. \end{cases} \tag{3.18}$$

By the invariance of the sets E_1, E_2, E_3, and E_4 under the translations of group T_{H_0}, the following equality holds for all $z \in G$ and $T \in T_{H_0}$:

$$f^{c,d}(T(z)) = f^{c,d}(z). \tag{3.19}$$

Definition 3.1. The notation being as above, let $a \in \mathbb{Z}^+$, $b \in \mathbb{Z}$, $N \in \mathbb{Z}^+ \cup \{\infty\}$. Define the equivalence relation $\sim(a, b, N) = \sim$ on G by

$$z \sim z' \Leftrightarrow z - z' \in H_N^{a,b}. \tag{3.20}$$

Remarks 3.1. Since $H_N^{a,b}$ is a subgroup of the abelian group G, it is a normal (invariant) subgroup of G. Thus, we can consider the quotient group $G/H_N^{a,b}$. The above equivalence relation is precisely the equivalence relation induced by the cosets of the quotient group $G/H_N^{a,b}$.

Definition 3.2. The notation being as above, let $a \in \mathbb{Z}^+$, $b \in \mathbb{Z}, c, d \in \mathbb{R}$, $N \in \mathbb{Z}^+ \cup \{\infty\}$. Let $\mu_N^{a,b,c,d} : G/\sim \to \mathbb{R}$ be the mapping defined by

$$\mu_N^{a,b,c,d}([z]) = f^{c,d}(z), \tag{3.21}$$

where $G/\sim$ stands for the set of all the equivalence classes of G generated by the equivalence relation $\sim$, and $[z]$ stands for the equivalence class containing z.

Remarks 3.2. The mapping $\mu_N^{a,b,c,d}$ can be equivalently defined on the quotient group $G/H_N^{a,b}$.

The fact that $\mu_N^{a,b,c,d}$ is well-defined easily follows from equation (3.19). We note that $\mu_\infty^{a,b,1,1}$ represents the nanotube(a, b) and that $\mu_N^{a,b,1,1}$ is the 'Nth approximation' of $\mu_\infty^{a,b,1,1}$, which converges to $\mu_\infty^{a,b,1,1}$ as $N \to \infty$ in a certain precise sense.

In this section, we have restricted the range of parameters c and d to $\mathbb{R}$, in order to keep a parallel between the notion of $\mu_N^{a,b,1,1}$ and its geometric picture obtained via the real-symmetric matrix representation of a labeled weighted graph. In sections 2, 6, and 7, the range of parameters c and d is set to be the complex field $\mathbb{C}$.

4. Adjacency matrix $K_N^{a,b,c,d}$ associated with $\mu_N^{a,b1,1}$, pseudo-circulant, and hyper-circulant

This section is a direct continuation of section 3.

Recall (3.1) and the fact that $z_1 = i$. Let

$$z' := z_1, \tag{4.1}$$

$$z'' := z_1 + i, \tag{4.2}$$

and let $N, a \in \mathbb{Z}^+$. We define a finite sequence $w_1, w_2, \ldots, w_{2aN}$ in $G = \mathbb{C}$ in two steps. This sequence is the main ingredient of definition 4.1 given below. Definition 4.1 is going to be used in theorem 4.1 which is central in this section.

First, using the translation operator T_p with $p \in G$, for each $j \in \{1, \ldots, a\}$ let

$$(w_{2j-1}, w_{2j}) := (T_{(j-1)u}(z'), T_{(j-1)u}(z'')), \tag{4.3}$$

where u is given by (3.4).

Second, using $w_1, w_2, \ldots, w_{2a}$ just defined above, for each $k \in \{1, \ldots, N-1\}$ let

$$(w_{1+2ak}, w_{2+2ak}, \ldots, w_{2a+2ak}) := (T_{kv}(w_1), T_{kv}(w_2), \ldots, T_{kv}(w_{2a})), \tag{4.4}$$

where v is given by (3.5).

Definition 4.1. The notation being as above, let

$$W := \{[w_1], [w_2], \ldots, [w_{2aN}]\}, \tag{4.5}$$

where $[w_j]$ denotes the equivalence class containing w_j. For each $x, y \in W$, let $d(x, y)$ denote the distance between the equivalence classes x and y:

$$d(x, y) := \inf\{|x' - y'| : x' \in x, y' \in y\}. \tag{4.6}$$

Remarks 4.1. It can be easily shown that the inf in (4.6) can be replaced by min and that $W = (W, d)$ forms a metric space. One can define a metric $\hat{d}$ on the quotient group $G/H_N^{a,b}$ similarly by considering the distance between cosets. Then, W is regarded as a metric subspace of the metric space $(G/H_N^{a,b}, \hat{d})$.

Theorem 4.1. The notation being as above, let $a \in \mathbb{Z}^+$ with $a \geqslant 2$, $b \in \mathbb{Z}$, $c = d = 1$, and let $N \in \mathbb{Z}^+$ with $N \geqslant 2$. Define the $2aN \times 2aN$ matrix $K_N^{a,b,c,d}$ by

$$(K_N^{a,b,c,d})_{st} = \begin{cases} 1 & \text{if } d([w_s], [w_t]) = 1, \\ 0 & \text{if } d([w_s], [w_t]) \neq 1. \end{cases} \tag{4.7}$$

Then, we have

$$K_N^{a,b,c,d} = L(N, a, -b, X, Y(c), Z(d)). \tag{4.8}$$

The matrix $K_N^{a,b,c,d}$ in theorem 4.1 can be regarded as the adjacency matrix of the molecular graph $\mathrm{Graph}_N^{a,b1,1}$ associated with $\mu_N^{a,b1,1}$. The molecular graph $\mathrm{Graph}_N^{a,b1,1}$ has $2aN$ labeled vertices $W = \{[w_1], [w_2], \ldots, [w_{2aN}]\}$ and the edges which reflect the adjacency relation defined by the criteria

$$d([w_s], [w_t]) = 1. \tag{4.9}$$

One can geometrically visualize $\mathrm{Graph}_N^{a,b1,1}$ by first rolling up the sheet of hexagons described by (3.13) so that Hex(0,0) is superimposed with Hex(a, b), and second by making the desired torus structure (that has N cyclic repetitions) out of the cylinder that has infinite translational repetitions.

Theorem 4.1 can be easily generalized to include the case in which a or N (or both) is equal to 1. In the present paper, however, we do not discuss this generalization since the new setting of the theory given in the next section does not require this extension.

It is convenient to introduce, at this moment, the following notions of an (m, n) pseudo-circulant, an (m, n) hyper-circulant, and an (m, n) block-diagonalizable matrix. The circulants and pseudo-circulants have been frequently used in the theories of hydrocarbons, polymers, and crystals (cf. [20,21]). Here, we shall newly establish the notion of an (m, n) hyper-circulant, which is a far reaching generalization of a circulant and a pseudo-circulant.

Definition 4.2. An $mn \times mn$ complex matrix A is called an (m, n) pseudo-circulant if there exist $Q_1, Q_2, \ldots, Q_m \in \boldsymbol{M}_n(\mathbb{C})$ such that

$$A = \begin{pmatrix} Q_m & Q_1 & Q_2 & \cdots & Q_{m-1} \\ Q_{m-1} & Q_m & Q_1 & \cdots & Q_{m-2} \\ Q_{m-2} & Q_{m-1} & Q_m & \cdots & Q_{m-3} \\ \vdots & \vdots & & & \vdots \\ Q_1 & Q_2 & \cdots & \cdots & Q_m \end{pmatrix}, \tag{4.10}$$

i.e., such that A can be expressed in terms of the jth power of the cyclic shift matrix P_m and the Kronecker product as follows

$$A = \sum_{j=1}^{m} P_m^j \otimes Q_j. \tag{4.11}$$

An $mn \times mn$ complex matrix A is called an (m, n) *hyper-circulant* if there exist $P \in \boldsymbol{M}_m(\mathbb{C})$, $Q_1, Q_2, \ldots, Q_m \in \boldsymbol{M}_n(\mathbb{C})$ such that P is semi-simple (diagonalizable) and such that

$$A = \sum_{j=1}^{m} P^j \otimes Q_j. \tag{4.12}$$

An $mn \times mn$ complex matrix A is called an (m, n) *block-diagonalizable matrix* if there exist $U \in \boldsymbol{M}_{mn}(\mathbb{C})$, $B_1, B_2, \ldots, B_m \in \boldsymbol{M}_n(\mathbb{C})$ such that U is non-singular and such that

$$U^{-1}AU = B\text{-diag}(B_1, B_2, \ldots, B_m), \tag{4.13}$$

where B-diag$(B_1, B_2, \ldots, B_m)$ denotes the $mn \times mn$ block-diagonal matrix in which the (j, j)th block is B_j and the (j, k)th block is the $n \times n$ zero matrix whenever $j \neq k$.

The following theorem provides the relation between (m, n) pseudo-circulants, (m, n) hyper-circulants, and (m, n) block-diagonalizable matrices. This theorem gives a guideline for solving problems (III) and (IV) formulated in section 6.

Theorem 4.2. Let $m, n \in \mathbb{Z}^+$. The following statements are true.

(i) If A is an (m, n) pseudo-circulant, then A is an (m, n) hyper-circulant.

(ii) If A is an (m, n) hyper-circulant, then A is an (m, n) block-diagonalizable matrix.

Proof. (i) The statement is true because the cyclic shift matrix P_m is unitary and hence semi-simple.

(ii) Assume that A is an (m, n) hyper-circulant. Then, there exist $P \in \boldsymbol{M}_m(\mathbb{C})$, $Q_1, Q_2, \ldots, Q_m \in \boldsymbol{M}_n(\mathbb{C})$ such that P is semi-simple and such that

$$A = \sum_{j=1}^{m} P^j \otimes Q_j. \tag{4.14}$$

Since P is semi-simple, there exists a nonsingular matrix $V \in \boldsymbol{M}_m(\mathbb{C})$ and a diagonal matrix $D \in \boldsymbol{M}_m(\mathbb{C})$ such that

$$V^{-1} P V = D. \tag{4.15}$$

By inserting $P = V D V^{-1}$ into (4.14), we have

$$\begin{aligned} A &= \sum_{j=1}^{m} (V D V^{-1})^j \otimes (I_n Q_j I_n) \\ &= \sum_{j=1}^{m} (V D^j V^{-1}) \otimes (I_n Q_j I_n) \\ &= \sum_{j=1}^{m} (V \otimes I_n)(D^j \otimes Q_j)(V^{-1} \otimes I_n) \\ &= (V \otimes I_n) \left(\sum_{j=1}^{m} D^j \otimes Q_j \right) (V^{-1} \otimes I_n). \end{aligned} \tag{4.16}$$

Bearing in mind the fact that $(V \otimes I_n)^{-1} = (V^{-1} \otimes I_n)$, we see that

$$\begin{aligned} (V \otimes I_n)^{-1} A (V \otimes I_n) &= \sum_{j=1}^{m} D^j \otimes Q_j \\ &= \text{B-diag} \left(\sum_{j=1}^{m} D_{11}^j Q_j, \sum_{j=1}^{m} D_{22}^j Q_j, \ldots, \sum_{j=1}^{m} D_{mm}^j Q_j \right). \end{aligned} \tag{4.17}$$

Therefore, A is (m, n) block-diagonizable. □

Definition 4.3. The procedure of block-diagonalization used in the proof of theorem 4.2 is referred to as the *Plug-in Block-diagonalization method for hyper-circulants*, or the *PB method*, for short.

Now we are ready to provide the

Proof of theorem 4.1. Put

$$n = a. \tag{4.18}$$

First, consider the case where $b = 0$. It is not difficult to check that $K_N^{n,0,c,d}$ is an $(N, 2n)$ pseudo-circulant of order $(2nN \times 2nN)$ given by

$$K_N^{n,0,c,d} = \begin{pmatrix} A_n & B_n & & & & & & B_n^* \\ B_n^* & A_n & B_n & & & & & \\ & B_n^* & A_n & B_n & & & & \\ & & B_n^* & \bullet & \bullet & & & \\ & & & \bullet & \bullet & \bullet & & \\ & & & & \bullet & \bullet & B_n & \\ & & & & & \bullet & A_n & B_n \\ B_n & & & & & & B_n^* & A_n \end{pmatrix}$$

$$= P_N^{-1} \otimes B_n^* + P_N^0 \otimes A_n + P_N^{+1} \otimes B_n, \tag{4.19}$$

where A_n and B_n are $2n \times 2n$ matrices given by

$$A_n = P_n^{-1} \otimes Y(c)^* + P_n^0 \otimes X + P_n^{+1} \otimes Y(c), \tag{4.20}$$

$$B_n = P_n^0 \otimes Z(d). \tag{4.21}$$

Notice also that A_n and B_n are $(n, 2)$ pseudo-circulants.

Second, consider the matrix $K_N^{n,b,c,d} - K_N^{n,0,c,d}$ and notice that it has the following $(N, 2n)$ pseudo-circulant form:

$$K_N^{n,b,c,d} - K_N^{n,0,c,d} = P_N^b \otimes C_n^* + P_N^0 \otimes (-C_n^* - C_n) + P_N^{-b} \otimes C_n, \tag{4.22}$$

where

$$C_n = (P_n S_n) \otimes Y(c). \tag{4.23}$$

The conclusion follows. □

Remarks 4.2. In equation (4.22), set $N = 8, b = 1$, for example, then $K_N^{n,b,c,d} - K_N^{n,0,c,d}$ has the following $(N, 2n)$ pseudo-circulant form:

$$K_N^{n,b,c,d} - K_N^{n,0,c,d} = \begin{pmatrix} D_n & C_n^* & & & & & & C_n \\ C_n & D_n & C_n^* & & & & & \\ & C_n & D_n & C_n^* & & & & \\ & & C_n & D_n & C_n^* & & & \\ & & & C_n & D_n & C_n^* & & \\ & & & & C_n & D_n & C_n^* & \\ & & & & & C_n & D_n & C_n^* \\ C_n^* & & & & & & C_n & D_n \end{pmatrix}, \quad (4.24)$$

where $D_n := -C_n^* - C_n$.

In the following sections, due to the notational convenience in using the RST, we frequently put $n = a$ and $t = -b$, where a and b are variables in the symbol nanotube (a, b). Notice that the block-matrix pattern in (4.24) with respect to the adjoint operation becomes the same as that of the block-matrix (4.19) if we consider $K_N^{n,-b,c,d} - K_N^{n,0,c,d}$ instead of $K_N^{n,b,c,d} - K_N^{n,0,c,d}$.

5. Standard alpha space $\mathscr{X}_{\#\alpha}(q, 1)$

The standard alpha space $\mathscr{X}_{\#\alpha}(q, 1)$ plays a major role in the present article. It is a special and important subset of the generalized repeat space $\mathscr{X}_r(q, d)$ which was defined in [4] for the first time.

Fix any $q \in \mathbb{Z}^+$, let $\{M_N\} = M_1, M_2, \ldots$ 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 $N \in \mathbb{Z}^+$,

$$M_N = \sum_{j=-v}^{v} P_N^j \otimes Q_j. \quad (5.1)$$

Then, $\{M_N\}$ 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 $\mathscr{X}_{\#\alpha}(q, 1)$.

If $\{M_N\} \in \mathscr{X}_{\#\alpha}(q, 1)$, then for any $N \in \mathbb{Z}^+$, M_N is an (N, q) pseudo-circulant, which can be easily demonstrated by using the fact that $P_N^j = P_N^k$ if $j \equiv k \pmod N$ and by recalling fundamental formulae for the Kronecker product, (2.12) and (2.13).

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

$$F(\theta) = \sum_{j=-v}^{v} (\exp(ij\theta)) Q_j. \quad (5.2)$$

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

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

$$Q_{-j} = Q_j^* \tag{5.3}$$

for all $j \in \{0, 1, \ldots, v\}$, and it follows that $F(\theta)$ defined by (5.2) is Hermitian for all $\theta \in \mathbb{R}$.

6. Formulation of problems

The eigenvalue problem of nanotube(a, b) in the Hückel crystal orbital scheme is equivalent to the eigenvalue problem of the Hermitian matrix-valued FS map $F^{a,-b,1,1}$ in the RST. In ref. [10], all the eigenvalues associated with this eigenvalue problem of nanotube (a, b) with $0 \leqslant b < a$ were given explicitly in a closed analytical form (cf. [10] and references therein). Thus, we see that all the eigenvalues of $F^{a,-b,1,1}(\theta)$ are explicitly obtainable if $0 \leqslant b < a$ and $\theta \in \mathbb{R}$. (Cf. remarks given below.)

Before formulating the problems, a few remarks must be made. We use the term 'generalized repeat space' in the formulation of problems (I) and (II) given below. At this moment however, it is not necessary for the reader to closely review the definition of this notion, which is given in the appendix. The generalized repeat space $\mathscr{X}_r(q, d)$ with block-size number q and dimension number d can be considered as a generalized analogue of the standard alpha space $\mathscr{X}_{\#\alpha}(q,\ 1)$ defined in section 5. Problems (I) and (II) concern the question of whether or not the sequences $\{M_N^{a,-b,c,d}\}_{N\in\mathbb{Z}^+}$ and $\{F^{n,-b,c,d}(\theta)\}_{n\in\mathbb{Z}^+}$ fall into a category of sequences which is central to and well-investigated in the RST.

Problems. Let $a \in \mathbb{Z}^+$, let $b \in \mathbb{Z}$, let $c, d \in \mathbb{C}$, and let $\theta \in \mathbb{R}$. Recall matrices $M_N^{n,t,c,d}$ and $F^{n,t,c,d}(\theta)$ defined by (2.25) and (2.26), respectively.

(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?

If these questions are answered affirmatively, then a new investigative link is formed, for the first time, between the research field of nanotubes and that

of the additivity, boundary effect, and other network problems, which had been investigated and solved using the RST. In this case, the mutual importation of theoretical notions and tools beyond the traditional research boundary becomes possible.

In section 7, we give affirmative answers to all of problems (I), (II), (III), and (IV).

Remarks 6.1. (1) If c_1 and c_2 are real numbers, and if L is an Hermitian matrix, then the eigenvalues of the Hermitian matrix $c_1 L^0 + c_2 L$ are given by $c_1 + c_2 \lambda_j(L)$ where $\lambda_j(L)$ denotes the jth eigenvalue of L.

(2) If H is the Hückel matrix of a conjugated molecule with the Coulomb integral α and the resonance integral β and if A is the adjacency matrix of the labeled graph of this molecule, then we have: $H = \alpha A^0 + \beta A$.

(3) The variable θ in the FS map is standard in the RST and this θ corresponds to a constant times the wave number vector k in ref. [10]; it has nothing to do with the conformational angle θ indicating the direction of the hexagon (a, b) in the graphite sheet defined in ref. [10].

7. Key theorems for the solutions of the problems

In this section, we establish key theorems 7.1, 7.2, 7.3, and 7.4 for the solutions of the problems formulated in section 6.

Theorem 7.1. The notation being as in section 2, we have

(I) The sequence $\{M_N^{a,-b,c,d}\}_{N\in Z^+}$ is an element of the generalized repeat space with size $(2a, 1)$.

(II) The sequence $\{F^{n,-b,c,d}(\theta)\}_{n\in Z^+}$ is an element of the generalized repeat space with size (2, 1).

Proof. (I) By the definition of $M_N^{a,-b,c,d}$, we easily see that

$$\{M_N^{a,-b,c,d}\}_{N\in Z^+} \in \mathscr{X}_{\#\alpha}(2a, 1). \tag{7.1}$$

By using equations (A.12), (A.13), and (A.14) in the appendix (review of the generalized repeat space), we get the relation

$$\mathscr{X}_{\#\alpha}(2a, 1) \subset \mathscr{X}_{\alpha}(2a, 1) \subset \mathscr{X}_{\alpha}(2a, 1) + \mathscr{X}_{\beta}(2a, 1) = \mathscr{X}_{r}(2a, 1), \tag{7.2}$$

so that we have

$$\{M_N^{a,-b,c,d}\}_{N\in Z^+} \in \mathscr{X}_{r}(2a, 1). \tag{7.3}$$

(II) Let

$$A_n := P_n^{-1} \otimes Y(c)^* + P_n^0 \otimes X + P_n^{+1} \otimes Y(c), \tag{7.4}$$

$$B_n := P_n^0 \otimes Z(d), \tag{7.5}$$

$$C_n := (P_n S_n) \otimes Y(c), \tag{7.6}$$

where $X, Y(c)$, and $Z(d)$ are given by (2.24). By using equations (A.12), (A.13), and (A.14) in the appendix, we can easily see that

$$\{A_n\}, \{B_n\}, \{C_n\} \in \mathscr{X}_r(2, 1). \tag{7.7}$$

On the other hand, by the definition of $F^{n,-b,c,d}(\theta)$, we have

$$\begin{aligned} F^{n,-b,c,d}(\theta) = \; & (e^{i\theta})^{-t} C_n^* + (e^{i\theta})^{-1} B_n^* + (e^{i\theta})^0 (A_n - C_n^* - C_n) \\ & + (e^{i\theta})^{+1} B_n + (e^{i\theta})^{+t} C_n. \end{aligned} \tag{7.8}$$

Theorem A.1 in the appendix implies that $\mathscr{X}_r(2, 1)$ is closed under the addition, multiplication, scalar multiplication, and $*$ operations. Therefore,

$$\{F^{n,-b,c,d}(\theta)\}_{n \in \mathbb{Z}^+} \in \mathscr{X}_r(2, 1). \tag{7.9}$$

□

Theorem 7.2. Let $q \in \mathbb{Z}^+$, let $\{A_N\} \in \mathscr{X}_{\#\alpha}(q, 1)$ be a standard alpha sequence with size $(q, 1)$. Suppose that A_N is Hermitian for all $N \in \mathbb{Z}^+$. Let F be the FS map associated with the sequence $\{A_N\}$. Let $h_j(\theta)$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with multiplicity, arranged in the increasing order $(1 \leqslant j \leqslant q)$. Then, for each $N \in \mathbb{Z}^+$, the following statements are true:

(i) A_N can be block-diagonalized as follows:

$$\begin{aligned} & (U_N \otimes I_q)^{-1} A_N (U_N \otimes I_q) \\ & = \text{B-diag}(F(2\pi/N), F(2\pi 2/N), \ldots, F(2\pi N/N)), \end{aligned} \tag{7.10}$$

where U_N denotes the $N \times N$ unitary matrix whose elements are

$$(U_N)_{mn} = N^{-1/2} \exp(2\pi mni/N), \tag{7.11}$$

I_q denotes the $q \times q$ identity matrix.

(ii) The eigenvalues of $qN \times qN$ Hermitian matrix A_N counted with multiplicity are:

$$h_1(2\pi 1/N), \ldots, h_1(2\pi N/N), \ldots, h_q(2\pi 1/N), \ldots, h_q(2\pi N/N). \tag{7.12}$$

(iii) For all $\theta \in \mathbb{R}$, we have

$$F(\theta + 2\pi) = F(\theta). \tag{7.13}$$

(iv) If $Q_{-v}, Q_{-v+1}, \ldots, Q_v$ are all real matrices, then for all $\theta \in \mathbb{R}$ we have

$$F(-\theta) = F(\theta)^T, \tag{7.14}$$

$$F(\pi - \theta) = F(\pi + \theta)^T, \tag{7.15}$$

$$\det(\lambda I_q - F(-\theta)) = \det(\lambda I_q - F(\theta)), \tag{7.16}$$

$$\det(\lambda I_q - F(\pi - \theta)) = \det(\lambda I_q - F(\pi + \theta)). \tag{7.17}$$

Proof. (i) By using the fundamental properties of the Kronecker product and the elementary equality for the diagonalization of P_N:

$$\begin{aligned} U_N^{-1} P_N U_N &= \operatorname{diag}(\exp(2\pi i/N), \exp(2\pi 2i/N), \ldots, \exp(2\pi Ni/N)) \\ &= D_N, \end{aligned} \tag{7.18}$$

equality (7.10) can be easily verified. In fact, by inserting $P_N = U_N D_N U_N^{-1}$ into $A_N = \sum_{j=-v}^{v} P_N^j \otimes Q_j$, one obtains

$$\begin{aligned} A_N &= \sum_{j=-v}^{v} (U_N D_N U_N^{-1})^j \otimes (I_q Q_n I_q) \\ &= (U_N \otimes I_q) \left(\sum_{j=-v}^{v} D_N^j \otimes Q_n \right) (U_N^{-1} \otimes I_q), \end{aligned} \tag{7.19}$$

from which (7.10) follows immediately.

(ii) This easily follows from (i).

(iii) Evident from the definition of F.

(iv) Assume that $Q_{-v}, Q_{-v+1}, \ldots, Q_v$ are all real matrices, and observe that

$$\begin{aligned} F(\theta) &= \sum_{j=-v}^{v} (\exp(-ij\theta)) Q_{-j} = \sum_{j=-v}^{v} (\exp(-ij\theta)) Q_j^T \\ &= \left(\sum_{j=-v}^{v} (\exp(-ij\theta)) Q_j \right)^T = F(-\theta)^T, \end{aligned} \tag{7.20}$$

and that

$$F(\pi - \theta) = F(-\pi + \theta)^T = F(\pi + \theta)^T. \tag{7.21}$$

The last two equalities in (iv) can be easily demonstrated by the fact that the determinant of matrix M is equal to the determinant of M^T.

□

Theorem 7.3. Recall the notation introduced in section 2 (definition of symbols), and set

$$q = rn, \tag{7.22}$$

$$A_N = L(N, n, t, x, y, z), \tag{7.23}$$

$$F(\theta) = \tilde{L}(\theta, n, t, x, y, z). \tag{7.24}$$

Let $h_j(\theta)$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with multiplicity, arranged in the increasing order ($1 \leqslant j \leqslant q$). Then, for each $N \in \mathbb{Z}^+$, the eigenvalues of $qN \times qN$ Hermitian matrix A_N counted with multiplicity are:

$$h_1(2\pi 1/N), \ldots, h_1(2\pi N/N), \ldots, h_q(2\pi 1/N), \ldots, h_q(2\pi N/N). \tag{7.25}$$

Proof. Note that $\{A_N\} \in \mathscr{X}_{\#\alpha}(q, 1)$ and that F is the FS map associated with the sequence $\{A_N\}$. The conclusion immediately follows from theorem 7.2. □

Definition 7.1. For each $n \in \mathbb{Z}^+$, let $\mathrm{Sg}_n : \{1, \ldots, 2n\} \to \{-1, 1\}$ denote the function defined by

$$\mathrm{Sg}_n(j) = \begin{cases} 1 & \text{if } j \in \{1, \ldots, n\}, \\ -1 & \text{if } j \in \{n+1, \ldots, 2n\}. \end{cases} \tag{7.26}$$

Theorem 7.4. The notation being as above, let $n \in \mathbb{Z}^+$, let $t \in \mathbb{Z}$, let $c, d \in \mathbb{C}$, and let $\theta \in \mathbb{R}$. Let

$$\rho := \rho(d, \theta) = 1 + d^* \exp(-i\theta). \tag{7.27}$$

Then, for $1 \leqslant j \leqslant 2n$, 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

$$\begin{aligned} \lambda_j^{n,t,c,d}(\theta) &= \mathrm{Sg}_n(j)\sqrt{|c|^2 + |\rho|^2 + 2\mathrm{Re}\left(c\rho \exp\left(i\left(\frac{t\theta + 2\pi j}{n}\right)\right)\right)} \\ &= \mathrm{Sg}_n(j)\sqrt{|c|^2 + |\rho|^2 + 2\,|c|\,|\rho| \cos\left(\mathrm{Arg}(c) + \mathrm{Arg}(\rho) + \frac{\theta t + 2\pi j}{n}\right)}. \end{aligned} \tag{7.28}$$

Proof. Let

$$\varepsilon := \varepsilon(t, \theta) = \exp(it\theta). \tag{7.29}$$

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

$$\hat{P}_n = \begin{pmatrix} 0 & 1 & & & & & \\ & 0 & 1 & & & \mathbf{0} & \\ & & 0 & \ddots & & & \\ & & & \ddots & \ddots & & \\ & & & & 0 & 1 & \\ & \mathbf{0} & & & & 0 & 1 \\ \varepsilon & & & & & & 0 \end{pmatrix}, \tag{7.30}$$

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

$$l^n - \varepsilon = 0, \tag{7.31}$$

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

$$l_j = \exp\left(i\left(\frac{t\theta + 2\pi j}{n}\right)\right), \tag{7.32}$$

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

$$\hat{D}_n := \mathrm{diag}(l_1, \ldots, l_n), \tag{7.33}$$

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

$$\hat{U}_n^{-1} \hat{P}_n \hat{U}_n = \hat{D}_n. \tag{7.34}$$

We mimic the argument in the proof of theorem 7.2(i), 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

$$F^{n,t,c,d}(\theta) = \sum_{k=-1}^{1} \hat{P}_n^k \otimes \hat{Q}_k, \tag{7.35}$$

where

$$\hat{Q}_{-1} = \begin{pmatrix} 0 & c^* \\ 0 & 0 \end{pmatrix}, \quad \hat{Q}_0 = \begin{pmatrix} 0 & \rho \\ \rho^* & 0 \end{pmatrix}, \quad \hat{Q}_1 = \begin{pmatrix} 0 & 0 \\ c & 0 \end{pmatrix}. \tag{7.36}$$

Now inserting $\hat{P}_n = \hat{U}_n \hat{D}_n \hat{U}_n^{-1}$ into equality (7.35), one obtains

$$F^{n,t,c,d}(\theta) = \sum_{k=-1}^{1} (\hat{U}_n \hat{D}_n \hat{U}_n^{-1})^k \otimes (I_2 \hat{Q}_k I_2)$$
$$= (\hat{U}_n \otimes I_2) \left(\sum_{k=-1}^{1} \hat{D}_n^k \otimes \hat{Q}_k \right) (\hat{U}_n^{-1} \otimes I_2). \tag{7.37}$$

Thus, $F^{n,t,c,d}(\theta)$ can be block-diagonalized as follows:

$$(\hat{U}_n \otimes I_2)^{-1} F^{n,t,c,d}(\theta)(\hat{U}_n \otimes I_2)$$
$$= \text{B-diag} \left(\sum_{k=-1}^{1} l_1^k \hat{Q}_k, \sum_{k=-1}^{1} l_2^k \hat{Q}_k, \ldots, \sum_{k=-1}^{1} l_n^k \hat{Q}_k \right). \tag{7.38}$$

By solving the characteristic equation of the jth diagonal block

$$\det \left(\lambda I_2 - \sum_{k=-1}^{1} l_j^k \hat{Q}_k \right) = \lambda^2 - (\rho + c^* l_j^{-1})(\rho^* + c l_j) = 0, \tag{7.39}$$

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

$$\pm\sqrt{|c|^2 + |\rho|^2 + 2\text{Re}(c\rho l_j)}$$
$$= \pm\sqrt{|c|^2 + |\rho|^2 + 2\text{Re}\left(c\rho \exp\left(i \left(\frac{t\theta + 2\pi j}{n} \right) \right) \right)}$$
$$= \pm\sqrt{|c|^2 + |\rho|^2 + 2\text{Re}\left(|c| \exp(i\,\text{Arg}(c))\, |\rho| \exp(i\,\text{Arg}(\rho)) \exp\left(i \left(\frac{t\theta + 2\pi j}{n} \right) \right) \right)}. \tag{7.40}$$

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

Now we can summarize the *Solutions of problems (I), (II), (III), and (IV)*. Problems (I), (II), (III), and (IV) formulated in section 6 have been all affirmatively solved by theorems 7.1, 7.2, 7.3, and 7.4: Problems (I) and (II) were solved by theorem 7.1. By theorem 7.3, the solution of problem (III) was reduced to that of problem (IV); one obtains the solution of problem (III) by combining theorems 7.3 and 7.4. Problem (IV) was solved by theorem 7.4.

As indicated earlier, the affirmative solutions of problems (I) and (II) form a new investigative link between the RST and the research field of nanotubes. Let us now utilize basic tools of the RST to see the reason why problems (III) and (IV) can be affirmatively solved. Since problem (III) can be reduced to problem (IV), we shall focus to problem (IV).

First, note that if $b = 0$, then we have

(i) $\{F^{n,-b,c,d}(\theta)\}_{n \in \mathbf{Z}^+} \quad \in \mathscr{X}_{\#\alpha}(2,1) \subset \mathscr{X}_r(2,1)$.

(ii) $F^{n,-b,c,d}(\theta)$ is an $(n, 2)$ pseudo-circulant for all $n \in \mathbb{Z}^+$.

(iii) $F^{n,-b,c,d}(\theta)$ is an $(n, 2)$ block-diagonalizable matrix for all $n \in \mathbb{Z}^+$.

Thus, if $b = 0$, by recalling (7.18) we can immediately see that all the eigenvalues of $F^{n,-b,c,d}(\theta)$ are explicitly obtainable by solving n quadratic equations.

Given any integer b, let us examine the property of the sequence $\{F^{n,-b,c,d}(\theta)\}_{n\in\mathbb{Z}^+}$ more closely than in the proof of theorem 7.1(II). Taking the nth power of both sides of (7.34), we obtain the relation

$$\hat{P}_n^n = \varepsilon I_n, \tag{7.41}$$

hence

$$\hat{P}_n^0 = (1/\varepsilon)\hat{P}_n^n, \tag{7.42}$$

$$\hat{P}_n^{-1} = (1/\varepsilon)\hat{P}_n^{n-1}. \tag{7.43}$$

Recalling formula (2.12) for the Kronecker product, and using (7.35), (7.42) and (7.43), we then have

$$F^{n,t,c,d}(\theta) = \hat{P}_n \otimes \hat{Q}_1 + \hat{P}_n^{n-1} \otimes ((1/\varepsilon)\hat{Q}_{-1}) + \hat{P}_n^n \otimes ((1/\varepsilon)\hat{Q}_0). \tag{7.44}$$

This implies that $F^{n,t,c,d}(\theta)$ is an $(n, 2)$ hyper-circulant with the semi-simple matrix $\hat{P}_n$ that satisfies (7.34).

It is easy to show that (7.38) and hence the conclusion of theorem 7.4 can also be obtained by strictly following the PB method described in definition 4.2. In fact, the method of the block-diagonalization employed in the proofs of theorems 7.2 and 7.4 is essentially the same as the PB method. The former method is an efficient variant of the PB method.

Thus, if b is any integer, then we have

(I) $\{F^{n,-b,c,d}(\theta)\}_{n\in\mathbb{Z}^+} \in \mathcal{X}_r(2, 1)$.

(II) $F^{n,-b,c,d}(\theta)$ is an $(n, 2)$ hyper-circulant with the semi-simple matrix $\hat{P}_n$ whose eigenvalues are analytically obtainable for all $n \in \mathbb{Z}^+$.

(III) $F^{n,-b,c,d}(\theta)$ is an $(n, 2)$ block-diagonalizable matrix for all $n \in \mathbb{Z}^+$, admitting the PB method and its variant method.

Consequently, in the general case in which b is any integer, we can also see the reason why all the eigenvalues of $F^{n,-b,c,d}(\theta)$ are explicitly obtainable. The classes of matrix sequences $\mathcal{X}_{\#\alpha}(2, 1)$ and $\mathcal{X}_r(2, 1)$ together with the notions of pseudo-circulants and hyper-circulants provide one with a comprehensive insight into the reason why problem (IV) can be solved affirmatively. Moreover, this insight naturally leads one to notice that in the repeat space $\mathcal{X}_r(q, d)$ with any positive block-size q and any positive dimension d, there exists a broad class of analytically diagonalizable matrix sequences that had been hitherto unknown.

Remarks 7.1. Since $\mathscr{X}_r(2,1)$ forms a $*$-algebra (cf. the appendix, theorem A.1), $\{F^{n,-b,c,d}(\theta)^2\}_{n\in Z^+} \in \mathscr{X}_r(2,1)$. The eigenvalue problems of matrices $F^{n,-b,c,d}(\theta)$ and $F^{n,-b,c,d}(\theta)^2$ can be simultaneously solved by using basic tools from the RST and theorem 2 from [22], which is a powerful tool for dealing with the problems of 'spectral symmetry' [23–28]. It has been confirmed that the formula (7.28) obtained in theorem 7.4 perfectly agrees with the formula obtained via the above-mentioned theorem of spectral symmetry. This theorem was initially established for the asymptotic analysis of a chemical kinetic dynamical system having a cyclic structure [22,27–29].

An ideal I of an algebra A is a nonempty subset of A that is both a linear subspace when A is considered as a linear space and an ideal when A is considered as a ring. For each $(q,d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$, the set $\mathscr{X}_\beta(q,d)$ defined by (A.11) in the appendix forms an ideal of the algebra $\mathscr{X}_r(q,d)$. For the proof of the fact that $\mathscr{X}_\beta(q,\ d)$ is a two-sided ideal of $\mathscr{X}_r(q,d)$, see ref. [6]. The ideal $\mathscr{X}_\beta(q,d)$ plays an important role in comparative studies of cyclic molecular networks having repeating identical moieties and their linear counterparts. We remark that the pseudo-circulant matrix sequence $\{M_N^{a,-b,c,d}\}_{N\in Z^+}$ in our theorem 7.1 can be used for a comparative study of toroidal carbon nanotubes (nanotori) and their linear counterparts when we consider the ideal $\mathscr{X}_\beta(2a,1)$. See [30–34] and references therein for recent studies of toroidal carbon nanotubes.

8. Application of the functional asymptotic linearity theorem to carbon nanotubes

In the repeat space theory (RST), the asymptotic linearity theorems (ALTs) play a central role in tackling a variety of additivity problems. The reader is referred to ref. [2] for various versions of the ALTs that prove the Fukui conjecture and solve the molecular additivity problems in a unifying manner. (For the methodology and examples of numerical analysis and computations of asymptotic quantities of alternant hydrocarbons, cf. [35,36] and references therein. For the definition of the original repeat space $X_r(q)$ with block-size q, cf. [2] and references therein.)

In this section, we provide the first application of the Functional ALT (the functional version of the ALT, proved in [2]) to carbon nanotubes. We formulate a problem, called 'problem γ', which involves a linear functional defined by using the assertion of the Functional ALT. A solution of problem γ shall be given at the end of this section after preparing essential preliminaries for the solution.

Fix any positive integer n, and fix any integer t. Let $\{M_N\} \in \mathscr{X}_{\#\alpha}(2n,1)$ be such that

$$M_N = L(N,n,t,X,Y(1),Z(1)) \tag{8.1}$$

for all $N \in \mathbb{Z}^+$, where L is given by (2.19); $X, Y(1)$, and $Z(1)$ are given by (2.24). Then, M_N is real-symmetric for all $N \in \mathbb{Z}^+$, and the sequence $\{M_N\}$ is an element of the original repeat space $X_r(2n)$ with block-size $2n$. Fix a closed interval I on the real line such that I contains all the eigenvalues of M_N for all $N \in \mathbb{Z}^+$. Let $AC(I)$ denote the normed space of all real-valued absolutely continuous functions on I equipped with the norm given by

$$||\varphi|| = \sup\{|\varphi(t)| : t \in I\} + V_I(\varphi), \tag{8.2}$$

where $V_I(\varphi)$ denotes the total variation of function φ. Let $AC(I)^*$ denote the dual space of $AC(I)$, in other words, let $AC(I)^*$ denote the real linear space of all the bounded linear functionals on $AC(I)$. Let $E_N : AC(I) \to \mathbb{R}$ denote the sequence of bounded linear functionals defined by

$$E_N(\varphi) := \mathrm{Tr}\varphi(M_N), \tag{8.3}$$

$N \in \mathbb{Z}^+$. [Cf. [2,5–8] for the definition of the 'function' of matrices $\varphi(M_N)$. Note that $\mathrm{Tr}\varphi(M_N) = \sum_{j=1}^{2nN} \varphi(\lambda_j(M_N))$, where $\lambda_j(M_N)$ denotes the jth eigenvalue of the real-symmetric matrix M_N counted with multiplicity, arranged in the increasing order.]

Then, the Functional ALT implies that there exist linear functionals $\alpha, \beta \in AC(I)^*$ such that

$$E_N(\varphi) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{8.4}$$

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

Define the sequence of linear functionals $\gamma_N : AC(I) \to \mathbb{R}$ by

$$\gamma_N(\varphi) = (E_N(\varphi) - (\alpha(\varphi)N + \beta(\varphi)))N, \tag{8.5}$$

$N \in \mathbb{Z}^+$. [Note that the Functional ALT implies that $\gamma_N \in AC(I)^*$ for every $N \in \mathbb{Z}^+$ and that $\gamma_N(\varphi) = o(N)$ as $N \to \infty$, for all $\varphi \in AC(I)$.]

For each nonnegative real number ξ, let $\varphi_\xi \in AC(I)$ denote the function defined by

$$\varphi_\xi(x) = |x|^\xi. \tag{8.6}$$

Then, the real number sequence $\{E_N(\varphi_1)\}, N \in \mathbb{Z}^+$, gives the sequence of the total pi-electron energy (TPEE) of the 'pseudo-circulant representation' of nanotube $(n, -t)$ with cluster size N. The real number sequence $\{E_N(\varphi_1 - \varphi_0)\}$, $N \in \mathbb{Z}^+$, gives the sequence of the delocalization energy (DE) of the 'pseudo-circulant representation' of nanotube $(n, -t)$ with cluster size N. [Note that $E_N(\varphi) = \alpha(\varphi)N + \beta(\varphi) + o(1)$ as $N \to \infty$, for all $\varphi \in \mathrm{span}\{\varphi_\xi : \xi \geqslant 0\} \subset AC(I)$.]

Since

$$E_N(\varphi_0) = 2nN \tag{8.7}$$

for all $N \in \mathbb{Z}^+$, we see that

$$\alpha(\varphi_0) = 2n, \tag{8.8}$$

$$\beta(\varphi_0) = 0, \tag{8.9}$$

hence that

$$\gamma_N(\varphi_0) = 0 \tag{8.10}$$

for all $N \in \mathbb{Z}^+$. By the linearity of the functional γ_N, we then have

$$\gamma_N(\varphi_1 - \varphi_0) = \gamma_N(\varphi_1) \tag{8.11}$$

for all $N \in \mathbb{Z}^+$.

Let $G : \mathbb{R} \to \mathbb{R}$ denote the function defined by

$$G(\theta) := \mathrm{Tr}\varphi_1(F(\theta)), \tag{8.12}$$

where F denotes the FS map associated with the sequence $\{M_N\}$, i.e.,

$$F(\theta) = \tilde{L}(\theta, n, t, X, Y(1), Z(1)), \tag{8.13}$$

and where $\tilde{L}$ is given by (2.23).

We are now ready to state problem γ.

Problem γ. Keep the notation and the assumptions as above. Describe the behavior of the real number sequence $\{\gamma_N(\varphi_1)\}$, which is equal to $\{\gamma_N(\varphi_1 - \varphi_0)\}$, in the following two cases:

$$\textbf{Case 1} : n + t \in 3\mathbb{Z}, \tag{8.14}$$

$$\textbf{Case 2} : n + t \notin 3\mathbb{Z}. \tag{8.15}$$

[Note: If one puts $a = n$ and $b = -t$, then $n + t \in 3\mathbb{Z}$ if and only if $2a + b \in 3\mathbb{Z}$. In ref. [10] and some other related references therein, the symbols a and b and the condition $2a + b \in 3\mathbb{Z}$ are used to discuss the conductivity of nanotubes. As mentioned earlier, here we use the variables n and t, which are more convenient in applying the RST to nanotubes.]

Preparation for answering problem γ. By the fundamental property of the FS map and by the fact that the matrices M_N are all real-symmetric, we know that $G : \mathbb{R} \to \mathbb{R}$ is a function that satisfies the following conditions

$$G(\theta + 2\pi) = G(\theta), \tag{8.16}$$

$$G(-\theta) = G(\theta), \tag{8.17}$$

for all $\theta \in \mathbb{R}$, which implies that

$$G(\pi - \theta) = G(\pi + \theta) \tag{8.18}$$

for all $\theta \in \mathbb{R}$.

Let $D^-G(\theta)$ and $D^+G(\theta)$ denote, respectively, the derivatives on the left and on the right at $\theta \in \mathbb{R}$:

$$D^-G(\theta) := \lim_{h \to -0} \frac{G(\theta + h) - G(\theta)}{h}, \tag{8.19}$$

$$D^+G(\theta) := \lim_{h \to +0} \frac{G(\theta + h) - G(\theta)}{h}, \tag{8.20}$$

and let

$$\delta^-(n, t) := D^-G\left(\frac{2\pi}{3}\right) = -D^+G\left(\frac{4\pi}{3}\right), \tag{8.21}$$

$$\delta^+(n, t) := D^+G\left(\frac{2\pi}{3}\right) = -D^-G\left(\frac{4\pi}{3}\right). \tag{8.22}$$

It is easy to show that for every $\theta \in \mathbb{R}$, both $D^+G(\theta)$ and $D^+G(\theta)$ exist in $\mathbb{R}$.

The following essential preliminaries given in (i)–(iv) form a basis for our solution of problem γ.

(i) In case 1, the function G is real-analytic thus differentiable everywhere except on the set

$$S := \{-2\pi/3, +2\pi/3\} + 2\pi\mathbb{Z}. \tag{8.23}$$

This can be demonstrated by directly computing $\delta^-(n, t)$ and $\delta^+(n, t)$ (see (8.28) and (8.29) below) and by noticing the fact that the function G is expressed in terms of the square root function and real-analytic functions $h_1, \ldots, h_n : \mathbb{R} \to \mathbb{R}$ as follows: $G(\theta) = \sum_{j=1}^{n} 2\sqrt{h_j(\theta)}$, where $h_j(\theta)$ is strictly positive for all $\theta \in \mathbb{R} - S$ and $j \in \{1, \ldots, n\}$.

Let

$$y_0 := 0, \tag{8.24}$$

$$y_1 := nu - tv, \tag{8.25}$$

$$y_2 := v, \tag{8.26}$$

$$y_3 := u, \tag{8.27}$$

where u and v are complex numbers defined by (3.4) and (3.5) respectively. Let ω denote the angle between the vectors $\overrightarrow{y_0y_1}$ and $\overrightarrow{y_0y_2}$ measured from the vector $\overrightarrow{y_0y_1}$. [*Remarks*: If one puts $a = n$ and $b = -t$, then $y_1 = au + bv$. Let Θ denote the angle between the vectors $\overrightarrow{y_0y_3}$ and $\overrightarrow{y_0y_1}$ measured from the vector $\overrightarrow{y_0y_3}$, then we have $\omega + \Theta = \pi/3$. In ref. [10] and some other related references therein, Θ is called the conformation angle.]

On the set S, the function G has cusps and the following equalities hold

$$\delta^-(n,t) = -2\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1} - \sqrt{3}\cot\left(\frac{\pi}{2n}\right), \tag{8.28}$$

$$\delta^+(n,t) = +2\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1} - \sqrt{3}\cot\left(\frac{\pi}{2n}\right), \tag{8.29}$$

$$\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1} = \frac{\sqrt{3}}{2\sin\omega}. \tag{8.30}$$

(ii) In case 2, G is real-analytic thus differentiable everywhere.

(iii) In this section, we assume the validity of the following statement, hypothesis I.

Hypothesis I. The notation and the assumptions being as above, we have for each $j = 0, 1,$ and 2,

$$\gamma_{3m+j}(\varphi_1) \to 2\pi \frac{B_2(j/3)}{2!} \int_0^{2\pi} G^{(2)}(\theta)\, d\theta \tag{8.31}$$

as $m \to \infty$.

For the proof of this hypothesis, one needs a special technique of asymptotic analysis, which is beyond the scope of this section. Here, we proceed taking this hypothesis for granted. See (9.17) in section 9, which is similar to (8.31) but is easy to prove.

Let B_2 denote the second Bernoulli function defined by

$$B_2(x) = x^2 - x + 1/6. \tag{8.32}$$

Then, in case 1, by using hypothesis I and the obvious relation

$$\int_0^{2\pi} G^{(2)}(\theta)\, d\theta = 2(\delta^-(n,t) - \delta^+(n,t)), \tag{8.33}$$

we have

$$\gamma_{3m+0}(\varphi_1) \to 2\pi B_2(0/3)(\delta^-(n,t) - \delta^+(n,t)), \tag{8.34}$$

$$\gamma_{3m+1}(\varphi_1) \to 2\pi B_2(1/3)(\delta^-(n,t) - \delta^+(n,t)), \tag{8.35}$$

$$\gamma_{3m+2}(\varphi_1) \to 2\pi B_2(2/3)(\delta^-(n,t) - \delta^+(n,t)), \tag{8.36}$$

as $m \to \infty$.

(iv) In case 2, we easily verify that

$$\delta^{-}(n,t) - \delta^{+}(n,t) = 0, \tag{8.37}$$

and that

$$\gamma_N(\varphi_1) \to 0 \tag{8.38}$$

as $N \to \infty$.

Define the oscillation of $\gamma_N(\varphi_1)$ by

$$\mathrm{Os}(\gamma_N(\varphi_1)) := \overline{\lim_{N\to\infty}}\, \gamma_N(\varphi_1) - \underline{\lim_{N\to\infty}}\, \gamma_N(\varphi_1). \tag{8.39}$$

With the above preparation we can now state the *Answer to problem* γ.

In case 1, the sequence $\gamma_N(\varphi_1)$ is divergent and

$$\gamma_{3m+0}(\varphi_1) \to -8\pi B_2(0/3)\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1}, \tag{8.40}$$

$$\gamma_{3m+1}(\varphi_1) \to -8\pi B_2(1/3)\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1}, \tag{8.41}$$

$$\gamma_{3m+2}(\varphi_1) \to -8\pi B_2(2/3)\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1}, \tag{8.42}$$

as $m \to \infty$. Since $B_2(0/3) = 1/6$, and $B_2(1/3) = B_2(2/3) = -1/18$, we have

$$\lim_{m\to\infty} \gamma_{3m+1}(\varphi_1) = \lim_{m\to\infty} \gamma_{3m+2}(\varphi_1), \tag{8.43}$$

and we also have

$$\begin{aligned}\mathrm{Os}(\gamma_N(\varphi_1)) &= \frac{16\pi}{9}\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1} \\ &= \frac{8\sqrt{3}\pi}{9\sin\omega}.\end{aligned} \tag{8.44}$$

In case 2,

$$\gamma_N(\varphi_1) \to 0 \tag{8.45}$$

as $N \to \infty$, and hence

$$\mathrm{Os}(\gamma_N(\varphi_1)) = 0. \tag{8.46}$$

We remark that the above analytical solution of problem γ has special physicochemical implications and prototypal importance in applying the RST to carbon nanotubes and related molecular networks, the detailed argument of which shall be published elsewhere.

To visualize the answer to problem γ and the asymptotic linearity of the sequence $E_N(\varphi_1)$, suppose that

$$n = 3, \tag{8.47}$$

$$t = -3, \tag{8.48}$$

so that $n + t = 0 \in 3\mathbb{Z}$, and let

$$c_0 := \lim_{m\to\infty} \gamma_{3m+0}(\varphi_1), \tag{8.49}$$

$$c_{1,2} := \lim_{m\to\infty} \gamma_{3m+1}(\varphi_1) = \lim_{m\to\infty} \gamma_{3m+2}(\varphi_1), \tag{8.50}$$

$$\mathrm{Os} := \mathrm{Os}(\gamma_N(\varphi_1)). \tag{8.51}$$

Then, we have

$$\sqrt{\left(\frac{t}{n}\right)^2 - \frac{t}{n} + 1} = \sqrt{3}, \tag{8.52}$$

$$\omega = \pi/6, \tag{8.53}$$

so that

$$c_0 = -8\pi(1/6)\sqrt{3}, \tag{8.54}$$

$$c_{1,2} = -8\pi(-1/18)\sqrt{3}, \tag{8.55}$$

$$\mathrm{Os} = \frac{16\sqrt{3}\pi}{9}. \tag{8.56}$$

Let us observe the results of the numerical computations given in figures 1 and 2, before proceeding to the next section.

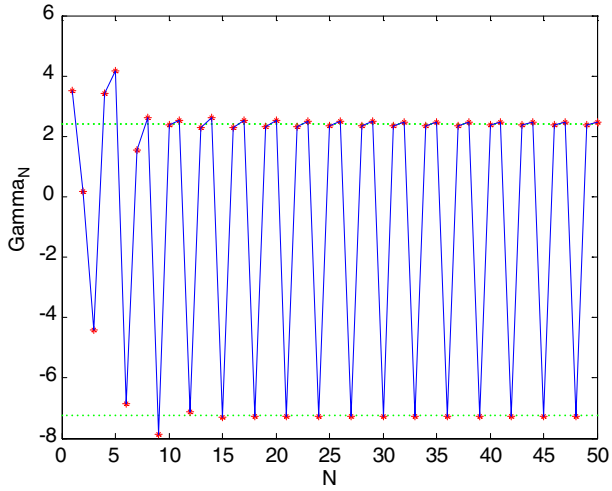

Figure 1. The plot of the sequence $\text{Gamma}_N := \gamma_N(\varphi_1) = \gamma_N(\varphi_1 - \varphi_0)$ and the theoretically obtained limits of the subsequences: $c_0 := \lim_{m\to\infty} \gamma_{3m+0}(\varphi_1)$ and $c_{1,2} := \lim_{m\to\infty} \gamma_{3m+1}(\varphi_1) = \lim_{m\to\infty} \gamma_{3m+2}(\varphi_1)$. The upper horizontal (dotted) line represents $c_{1,2}$ and the lower horizontal (dotted) line represents c_0. The oscillation of the sequence $\gamma_N(\varphi_1)$ is the distance between these two lines, which is $16\sqrt{3}\pi/9$.

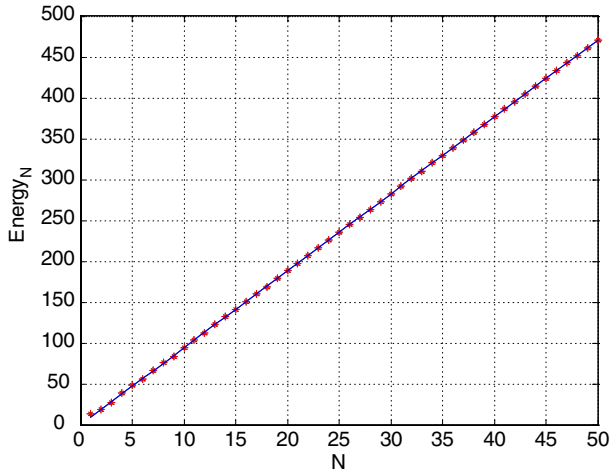

Figure 2. The plot of the TPEE $\text{Energy}_N := E_N(\varphi_1)$ of the pseudo-circulant representation of nanotube(3, 3) with cluster size N. The stars * represent the numerically computed $E_N(\varphi_1)$ and the line to which the point $\text{Pt}_N := (N, E_N(\varphi_1)) \in \mathbb{R}^2$ rapidly approaches is the asymptotic line $\alpha(\varphi_1)N + \beta(\varphi_1)$ which the Functional ALT predicts in a broader context.

9. Application of the functional asymptotic linearity theorem to monocyclic polyenes

In this section, we present the first application of the Functional ALT to the monocyclic conjugated polyenes $C_{2N}H_{2N}$, $N \in \{2, 3, \ldots\}$, whose Hückel adjacency matrix is given by setting $c = 0$ and $d = 1$ in (2.24) and by using our formula (2.19) in section 2.

Let $\{A_N\} \in \mathscr{X}_{\#\alpha}(2, 1)$ be such that

$$A_N = L(N, 1, 0, X, Y(0), Z(1)) \tag{9.1}$$

for all $N \in \mathbb{Z}^+$, where L is given by (2.19); X, $Y(0)$, and $Z(1)$ are given by (2.24). Then, A_N is real-symmetric for all $N \in \mathbb{Z}^+$, and the sequence $\{A_N\}$ is an element of the original repeat space $X_r(2)$ with block-size 2. Fix a closed interval I on the real line such that I contains all the eigenvalues of A_N for all $N \in \mathbb{Z}^+$.

Let e_N: $AC(I) \to \mathbb{R}$ denote the sequence of bounded linear functionals defined by

$$e_N(\varphi) := \mathrm{Tr}\varphi(A_N), \tag{9.2}$$

$N \in \mathbb{Z}^+$. [Note: Throughout this section, we let the domain of the sequence e_N be the set of all positive integers $\mathbb{Z}^+$. We do not restrict the domain to the set $\{2, 3, \ldots\}$.]

Then, the Functional ALT implies that there exist linear functionals α, $\beta \in AC(I)^*$ such that

$$e_N(\varphi) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{9.3}$$

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

Define the sequence of linear functionals $\gamma_N^A : AC(I) \to \mathbb{R}$ by

$$\gamma_N^A(\varphi) = (e_N(\varphi) - (\alpha(\varphi)N + \beta(\varphi)))N, \tag{9.4}$$

$N \in \mathbb{Z}^+$. [Note that the Functional ALT implies that $\gamma_N^A \in AC(I)^*$ for every $N \in \mathbb{Z}^+$ and that $\gamma_N^A(\varphi) = o(N)$ as $N \to \infty$, for all $\varphi \in AC(I)$.] For each nonnegative real number ξ, let $\varphi_\xi \in AC(I)$ denote the function defined by

$$\varphi_\xi(x) = |x|^\xi. \tag{9.5}$$

Then, the real number sequence $\{e_N(\varphi_1)\}$, $N \in \{2, 3, \ldots\}$, gives the sequence of the total pi-electron energy (TPEE) of $C_{2N}H_{2N}$. The real number sequence $\{e_N(\varphi_1 - \varphi_0)\}$, $N \in \{2, 3, \ldots\}$, gives the sequence of the delocalization energy (DE) of $C_{2N}H_{2N}$. [Note that $e_N(\varphi) = \alpha(\varphi)N + \beta(\varphi) + o(1)$ as $N \to \infty$, for all $\varphi \in \mathrm{span}\,\{\varphi_\xi : \xi \geqslant 0\} \subset AC(I)$.]

Since

$$e_N(\varphi_0) = 2N \tag{9.6}$$

for all $N \in \mathbb{Z}^+$, we see that

$$\alpha(\varphi_0) = 2, \tag{9.7}$$

$$\beta(\varphi_0) = 0, \tag{9.8}$$

hence that

$$\gamma_N^A(\varphi_0) = 0 \tag{9.9}$$

for all $N \in \mathbb{Z}^+$. By the linearity of the functional γ_N^A, we then have

$$\gamma_N^A(\varphi_1 - \varphi_0) = \gamma_N^A(\varphi_1) \tag{9.10}$$

for all $N \in \mathbb{Z}^+$.

Let g: $\mathbb{R} \to \mathbb{R}$ denote the function defined by

$$g(\theta) := \mathrm{Tr}\varphi_1(f(\theta)), \tag{9.11}$$

where f denotes the FS map associated with the sequence $\{A_N\}$, i.e.,

$$f(\theta) = \tilde{L}(\theta, 1, 0, X, Y(0), Z(1)), \tag{9.12}$$

where $\tilde{L}$ is given by (2.23). [Note: The function $g(\theta)$ is expressed in terms of the eigenvalues of the 2×2 matrix $f(\theta)$, as $g(\theta) = \mathrm{Tr}\varphi_1(f(\theta)) = \sum_{j=1}^{2} |\lambda_j(f(\theta))|$, where $\lambda_j(f(\theta))$ denotes the jth eigenvalue of the Hermitian matrix $f(\theta)$ counted with multiplicity, arranged in the increasing order.]

We formulate a problem, called 'problem γ^A', which is analogous to problem γ in section 8 but is simpler than problem γ.

Problem $\boldsymbol{\gamma^A}$. Keep the notation and the assumptions as above. Describe the behavior of the real number sequence $\{\gamma_N^A(\varphi_1)\}$, which is equal to $\{\gamma_N^A(\varphi_1 - \varphi_0)\}$.

The following proposition provides an answer to this problem.

Proposition 9.1. The notation and the assumptions being as above, suppose that φ is either φ_1 or $\varphi_1 - \varphi_0$. Then, we have

$$\gamma_{2m+0}^A(\varphi) \to -4\pi B_2(0/2) = -2\pi/3, \tag{9.13}$$

$$\gamma_{2m+1}^A(\varphi) \to -4\pi B_2(1/2) = \pi/3, \tag{9.14}$$

as $m \to \infty$, and

$$\mathrm{Os}(\gamma_N^A(\varphi)) := \overline{\lim_{N\to\infty}} \gamma_N^A(\varphi) - \underline{\lim_{N\to\infty}} \gamma_N^A(\varphi) = \pi, \tag{9.15}$$

where B_2 denotes the second Bernoulli function, $B_2(x) = x^2 - x + 1/6$.

Proof. In view of equality (9.10), we may and do assume that $\varphi = \varphi_1$. By using theorem 7.4, we readily see that

$$g(\theta) = 4\left|\cos\frac{\theta}{2}\right| \tag{9.16}$$

for all $\theta \in \mathbb{R}$. Apply the Euler–Maclaurin formula that uses the Bernoulli functions $B_n(x)$ (cf. [37,38] and references therein) to the restriction of the function g to the closed interval $[-\pi, \pi]$, so that we have for each $j = 0$ and 1,

$$\gamma^A_{2m+j}(\varphi_1) \to 2\pi\frac{B_2(j/2)}{2!}\int_0^{2\pi} g^{(2)}(\theta)\,d\theta \tag{9.17}$$

as $m \to \infty$. But, we have

$$\int_0^{2\pi} g^{(2)}(\theta)\,d\theta = D^- g\left(\frac{2\pi}{2}\right) - D^+ g\left(\frac{2\pi}{2}\right) = -4, \tag{9.18}$$

$$B_2(0/2) = 1/6, \tag{9.19}$$

$$B_2(1/2) = -1/12. \tag{9.20}$$

The conclusion follows. □

The numerical computation of $\gamma^A_N(\varphi_1)$ shows that the sequence $\gamma^A_N(\varphi_1)$ begins to oscillate immediately and the subsequences $\gamma^A_{2m+0}(\varphi_1)$ and $\gamma^A_{2m+1}(\varphi_1)$ begins to converge rapidly as figure 3 shows.

The behavior of the sequence $\{\gamma^A_N(\varphi_1)\} = \{\gamma^A_N(\varphi_1 - \varphi_0)\}$ implies that $C_{2N}H_{2N}$ with $N = 2m+1$ are relatively more stable than $C_{2N}H_{2N}$ with $N = 2m$, although this relative stability decreases as N becomes larger. See figure 4, which shows that the point $\mathrm{Pt}_N := (N, e_N(\varphi_1)) \in \mathbb{R}^2$ rapidly approaches the asymptotic line $\alpha(\varphi_1)N + \beta(\varphi_1)$. Recall (9.7) and (9.8), and notice that in the plot of the delocalization energy of $C_{2N}H_{2N}$, the point $\mathrm{Pt}^D_N := (N, e_N(\varphi_1 - \varphi_0)) \in \mathbb{R}^2$ rapidly approaches its asymptotic line:

$$\alpha(\varphi_1 - \varphi_0)N + \beta(\varphi_1 - \varphi_0) = (\alpha(\varphi_1) - 2)N + \beta(\varphi_1). \tag{9.21}$$

Proposition 9.1 and the plot in figure 3 provide a fresh insight into Hückel's $(4n + 2)$ rule concerning the aromaticity of monocyclic polyenes.

The oscillation of $\gamma^A_N(\varphi_1)$, or the oscillation of $\gamma^A_N(\varphi_1 - \varphi_0)$, is the positive number π. This implies that the pi-electron energy band structure of polyacetylene (calculated via the Hückel scheme without bond alternation) has the zero-band gap.

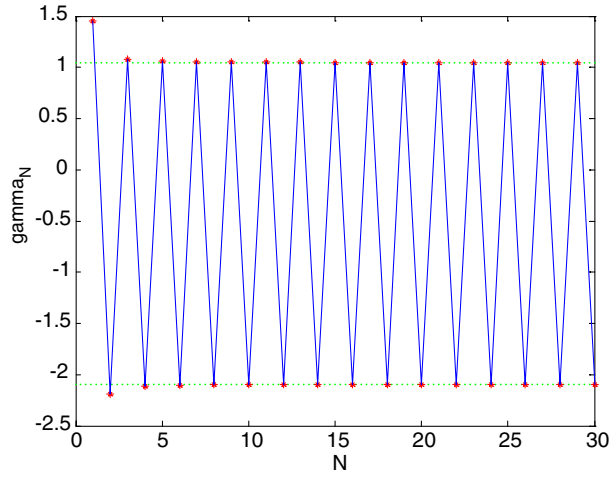

Figure 3. The plot of the sequence $\text{gamma}_N := \gamma_N^A(\varphi_1) = \gamma_N^A(\varphi_1 - \varphi_0)$ and the theoretically obtained limits of the subsequences: $\lim_{m\to\infty} \gamma_{2m+0}^A(\varphi_1) = -2\pi/3$ and $\lim_{m\to\infty} \gamma_{2m+1}^A(\varphi_1) = \pi/3$. The upper horizontal (dotted) line represents $\pi/3$ and the lower horizontal (dotted) line represents $-2\pi/3$. The oscillation of the sequence $\gamma_N^A(\varphi_1)$ is the distance between these two lines, which is π.

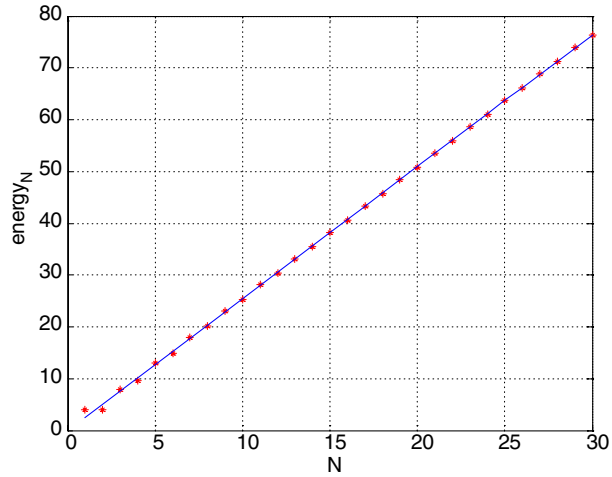

Figure 4. The plot of the TPEE $\text{energy}_N := e_N(\varphi_1)$ of monocyclic polyene $C_{2N}H_{2N}$ ($N \in \{2, 3, \ldots\}$) and the asymptotic line of the energy. The stars $*$ represent the numerically calculated $e_N(\varphi_1)$ and the line to which the point $\text{Pt}_N := (N, e_N(\varphi_1)) \in \mathbb{R}^2$ rapidly approaches is the asymptotic line $\alpha(\varphi_1)N + \beta(\varphi_1)$ which the Functional ALT predicts in a broader context.

The detailed discussion of the application of the ALT along these lines shall be published elsewhere.

10. Concluding remarks

In the present paper, we used the following two distinct but complementary research modes (strategies):

(1) '*global contextualization of molecular problems*' expounded in ref. [1] entitled 'Note on the repeat space theory – its development and communication with Prof. Kenichi Fukui-',

(2) '*local analysis of prototypal concrete problems*' of nanotubes and monocyclic polyenes.

We subsumed the nanotube problem under the operator-theoretic setting of the RST, namely under the structure of the $*$-algebra of the repeat space $\mathcal{X}_r(q, 1)$. Through this global contextualization, we obtained among other things:

(i) the analytic expressions for the spectra of nanotube$[a, b, c, d]$ with cluster size N,

(ii) the analytic expressions for the energy band curves of nanotube$[a, b, c, d]$,

where nanotube$[a, b, c, d]$ denotes our sequential matrix representation of nanotube(a, b) with the complex variables c and d. Also through this global contextualization, all the theoretical tools and theorems in papers [7,8] are now applicable to nanotube$[a, b, c, d]$ with cluster size N so that we can investigate the additivity and reactivity quantities (such as the frontier electron density, superdelocalizability) of nanotubes in a unifying manner.

Concerning (2): This research mode corresponds to sections 8 and 9 in the present paper, although these sections partially utilize the global setting of the RST. Sections 8 and 9 are, both from a mathematical and chemical point of view, as important as the preceding sections. Note that the asymptotic linearity theorem (ALT) is used in conjunction with the notion of the ***electron delocalization*** – the central concept of the frontier orbital theory [7,8]. Also note that our answer to problem γ gives, in conjunction with the ALT, a necessary and sufficient condition for the pi-electron band curves of nanotube(a, b) to have the zero-band gap, which is an important criterion of the metallic conductivity. The notion of the electron delocalization thus used enriches our line of research a great deal and enhances the development of the RST, which now uses the theory of algebraic and analytic curves, and resolution of singularities [14,15].

Appendix. Review of the generalized repeat space

There are several equivalent ways of defining the generalized repeat space $\mathscr{X}_r(q,d)$ with a given size $(q,d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$. We shall recall below the definition that uses the notion of the sum of subspaces of a linear space (cf. refs. [4,6,7]).

Fix $(q,d) \in \mathbb{Z}^+ \times \mathbb{Z}^+$ and let $\mathscr{X}(q,d)$ denote the set of all matrix sequences whose Nth 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

$$\{M_N\} + \{M'_N\} = \{M_N + M'_N\}, \tag{A.1}$$

$$k\{M_N\} = \{kM_N\}, \tag{A.2}$$

$$\{M_N\}\{M'_N\} = \{M_N M'_N\}, \tag{A.3}$$

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

$$\{M_N\}^* = \{M_N^*\}, \tag{A.4}$$

where the * on the right-hand side of (A.4) denotes the adjoint operation.

Let P_N^n denote the $N^d \times N^d$ matrix given by

$$P_N^n = P_N^{n_1} \otimes P_N^{n_2} \otimes \ldots \otimes P_N^{n_d}, \tag{A.5}$$

where $n = (n_1, n_2, \ldots, n_d) \in \mathbb{Z}^d$, and $\otimes$ denotes the Kronecker product.

Let S_N^k denote the $N^d \times N^d$ matrix given by

$$S_N^k = S_N^{k_1} \otimes S_N^{k_2} \otimes \ldots \otimes S_N^{k_d}, \tag{A.6}$$

where $k = (k_1, k_2, \ldots, k_d) \in (\mathbb{Z}^+ \cup \{0\})^d$.

Let $\mathcal{V}^k(q,d)$ with $k = (k_1, k_2, \ldots, k_d) \in \{0,1\}^d$ denote the subset of $\mathscr{X}(q,d)$ defined by

$$\begin{aligned}\mathcal{V}^k(q,d) = \{\{M_N\} \in \mathscr{X}(q,d) : \exists m, n \in \mathbb{Z}^d, \exists Q \in \boldsymbol{M}_q(\mathbb{C}) \text{ such that} \\ M_N = (P_N^m S_N^k P_N^n) \otimes Q \text{ for all } N \gg 0\}.\end{aligned} \tag{A.7}$$

Let span $\mathcal{V}^k(q,d)$ with $k = (k_1, k_2, \ldots, k_d) \in \{0,1\}^d$ denote the linear span of $\mathcal{V}^k(q,d)$.

We define three fundamental linear subspaces

$\mathscr{X}_r(q,d), \mathscr{X}_\alpha(q,d),$ and $\mathscr{X}_\beta(q,d)$ of $\mathscr{X}(q,d)$ by

$$\mathscr{X}_r(q,d) = \sum_{k\in\{0,1\}^d} \text{span } \mathcal{V}^k(q,d), \tag{A.8}$$

$$\mathscr{X}_\alpha(q,d) = \text{ span } \mathcal{V}^{\mathbf{0}}(q,d), \tag{A.9}$$

$$\text{where } \mathbf{0} = (0,0,\ldots,0) \in \{0,1\}^d, \tag{A.10}$$

$$\mathscr{X}_\beta(q,d) = \sum_{k\in\{0,1\}^d\setminus\{\mathbf{0}\}} \text{span } \mathcal{V}^k(q,d). \tag{A.11}$$

In (A.8) and (A.11), the Σ denotes the sum of subspaces in the obvious manner.

We call $\mathscr{X}_r(q,d), \mathscr{X}_\alpha(q,d), \mathscr{X}_\beta(q,d)$, respectively, the generalized repeat space, generalized alpha space, and generalized beta space with size (q,d), and each element of $\mathscr{X}_r(q,d), \mathscr{X}_\alpha(q,d), \mathscr{X}_\beta(q,d)$, respectively, a generalized repeat sequence, generalized alpha sequence, and generalized beta sequence with size (q,d).

The following is one of the most fundamental theorems in the repeat space theory.

Theorem A.1. For all $q,d \in \mathbb{Z}^+$, $\mathscr{X}_r(q,d)$ forms a $*$-algebra.

Proof. This was proved in ref. [6]. □

For the purpose of the present article, in which only the generalized repeat space with size $(q,1)$ appears, set $d=1$ in the definition of $\mathcal{V}^k(q,d)$ given by (A.7) and observe that

$$\begin{aligned}\mathscr{X}_\alpha(q,1) &= \text{span}\mathcal{V}^0(q,1)\\ &= \text{span}\{\{M_N\}\in\mathscr{X}(q,1) : \exists m\in\mathbb{Z}, \exists Q\in \boldsymbol{M}_q(\mathbb{C}) \text{ such that}\\ &\qquad M_N = P_N^m \otimes Q \text{ for all } N\gg 0\},\end{aligned} \tag{A.12}$$

$$\begin{aligned}\mathscr{X}_\beta(q,1) &= \text{ span } \mathcal{V}^1(q,1)\\ &= \text{ span } \{\{M_N\}\in\mathscr{X}(q,1) : \exists m,n\in\mathbb{Z}, \exists Q\in \boldsymbol{M}_q(\mathbb{C}) \text{ such that}\\ &\qquad M_N = (P_N^m S_N P_N^n)\otimes Q \text{ for all } N\gg 0\},\end{aligned} \tag{A.13}$$

and note that

$$\mathscr{X}_r(q,1) = \mathscr{X}_\alpha(q,1) + \mathscr{X}_\beta(q,1). \tag{A.14}$$

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