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New proof of the Fukui conjecture by the Functional Asymptotic Linearity Theorem

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Dedicated to the memory of Professor Kenichi Fukui (1918–1998)

The present article provides a new proof of the Fukui conjecture concerning the additivity problem of the zero-point vibrational energies of hydrocarbons. This conjecture played a prominent role in the initial development of the repeat space theory (RST), and continues to be of vital significance in the recent development of the theory of the generalized repeat space $\mathscr{X}_r(q, d)$. The new proof of the Fukui conjecture has been given here by establishing the functional version of the Asymptotic Linearity Theorem (ALT), the Functional ALT. This enhanced version of the ALT directly implies the validity of the Fukui conjecture; it easily unifies, in a broad perspective, a variety of additivity phenomena in physico-chemical network systems having many identical moieties, and efficiently solves some interpretational problems of the empirical additivity formulae from experimental chemistry. The proof of the functional version of the ALT is based on a new method transferable to the extended theoretical framework of the generalized repeat space $\mathscr{X}_r(q, d)$.

KEY WORDS: Fukui conjecture, repeat space theory (RST), additivity problems, Asymptotic Linearity Theorem (ALT)

1. Introduction

In his later years, Kenichi Fukui (1918–1998) presented several conjectures concerning the additivity problems of molecules having many identical moieties. Among them is the following which has been playing a significant role in the development of the repeat space theory (RST).

Fukui's conjecture on the zero-point energy additivity. A theoretical foundation for the empirical additive formulae for the zero-point vibrational energy of hydrocarbons will be laid in a general mathematical theory by which one can prove the following proposition.

Proposition I. Let $\{M_N\}$ be a fixed element of the repeat space with block-size q, and let I be a fixed closed interval on the real line such that I contains all the eigenvalues

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of M_N for all positive integers N. Let $\varphi_{1/2}: I \to \mathbb{R}$ denote the function defined by $\varphi_{1/2}(t) = |t|^{1/2}$. Then, there exist real numbers α and β such that

$$\mathrm{Tr}\,\varphi_{1/2}(M_N) = \alpha N + \beta + o(1) \tag{1.1}$$

as $N \to \infty$.

In the present article, the mathematical part of Fukui's conjecture on the zero-point energy additivity, namely proposition I, shall be referred to as "the Fukui conjecture".

The main purpose of this article is to give a new proof of the Fukui conjecture by what we call the functional version of the Asymptotic Linearity Theorem (ALT), or the Functional ALT for short. This theorem has first been presented in [1], however, its proof was yet to be made public. The present article publicizes, for the first time, a detailed proof of the Functional ALT. This enhanced version of the ALT directly implies the validity of the Fukui conjecture; it easily unifies, in a broad perspective, a variety of additivity phenomena in physico-chemical network systems having many identical moieties, and efficiently solves some interpretational problems of the empirical additivity formulae from experimental chemistry (cf. the preceding article [2, sections 2 and 3]).

The investigations of the vibrational energy additivity of hydrocarbons have a history of several decades. To understand the origin and development of the research of vibrational energy additivity problems, which are closely related to thermodynamic additivity problems, the reader is referred to the phenomenological studies of experimental chemists (cf. [3–7] and references therein). The reader is also referred to investigations of the additivity problems of the total pi electron energies [8–21], which had long been investigated separately from the vibrational energy additivity problems of hydrocarbons until the notion of the repeat space (with block-size q) $X_r(q)$ was utilized.

In section 2, we review the notion of the repeat space (with block-size q) $X_r(q)$, and in section 3, chronologically review the ALTs that imply the Fukui conjecture. In section 4, we formulate a problem whose solution, by what we call the Compatibility Theorem, streamlines the proof process of all the different versions of the ALT. Section 5 provides a proof of the Functional ALT assuming the validity of the Compatibility Theorem. Section 6 establishes the notion of standard alpha space (with block-size q) $X_{\#\alpha}(q)$ and prepares other preliminaries for the Compatibility Theorem whose proof is given in section 7.

2. Review of the repeat space $X_r(q)$

Throughout, let $\mathbb{Z}^+$, $\mathbb{R}$, and $\mathbb{C}$ denote respectively the set of all positive integers, real numbers, and complex numbers; and the symbol $\mathbb{K}$ will denote either $\mathbb{R}$ or $\mathbb{C}$. By "for all $N \gg 0$", we mean "for all positive integers N greater than some given positive integer".

In what follows, we review the notion of the repeat space (with block-size q) $X_r(q)$, according to [22] in which this notion was first established. We remark that the repeat space $X_r(q)$ can be also defined within the framework of the extended setting of the generalized repeat space $\mathscr{X}_r(q, d)$ (cf. [1]).

Fix a $q \in \mathbb{Z}^+$, and let $X(q)$ denote the set of all matrix sequences whose Nth term M_N is an arbitrary $qN \times qN$ real symmetric matrix, $N \in \mathbb{Z}^+$. This set obviously constitutes a linear space over the field $\mathbb{R}$ with term-wise addition and scalar multiplication

$$\{M_N\} + \{M'_N\} = \{M_N + M'_N\}, \tag{2.1}$$

$$k\{M_N\} = \{kM_N\}, \tag{2.2}$$

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

We defined three fundamental linear subspaces $X_r(q)$, $X_\alpha(q)$, and $X_\beta(q)$ of $X(q)$. The subspace $X_r(q)$ is defined to be the set of all matrix sequences $\{M_N\} \in X(q)$ such that for all $N \gg 0$,

$$M_N = A_N + B_N, \tag{2.3}$$

where A_N, B_N are $qN \times qN$ real matrices having the partitioned forms given below:

$$A_N = \begin{pmatrix}
Q_0 & Q_1 & \cdot & \cdot & Q_\nu & & & & Q_{-\nu} & \cdot & Q_{-2} & Q_{-1} \\
Q_{-1} & Q_0 & Q_1 & \cdot & \cdot & Q_\nu & & & & \cdot & \cdot & Q_{-2} \\
\cdot & Q_{-1} & \cdot & \cdot & \cdot & \cdot & \cdot & & & & Q_{-\nu} & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \mathbf{0} & & Q_{-\nu} \\
Q_{-\nu} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & \\
 & Q_{-\nu} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \\
 & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & Q_\nu & \\
 & & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & Q_\nu \\
Q_\nu & & \mathbf{0} & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & & & & \cdot & \cdot & \cdot & \cdot & \cdot & Q_1 & \cdot \\
Q_2 & \cdot & Q_\nu & & & & Q_{-\nu} & \cdot & \cdot & Q_{-1} & Q_0 & Q_1 \\
Q_1 & Q_2 & \cdot & Q_\nu & & & & Q_{-\nu} & \cdot & \cdot & Q_{-1} & Q_0
\end{pmatrix}, \tag{2.4}$$

where ν is a nonnegative integer, $Q_{-\nu}, Q_{-\nu+1}, \ldots, Q_\nu$ are $q \times q$ real matrices, ν and Q_n are constant and independent of N. A_N is defined for all $N \in \mathbb{Z}^+$ with $N > 2\nu + 1$. (Note that Q_{-n} is the transpose of Q_n for all $n \in \{0, 1, \ldots, \nu\}$.)

For all $N \gg 0$, we can equivalently write A_N in a concise form:

$$A_N = \sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n, \tag{2.5}$$

where P_N denotes an $N \times N$ real-orthogonal matrix given by

$$P_N = \begin{pmatrix}
0 & 1 & 0 & \ldots & 0 \\
0 & 0 & 1 & \ddots & \vdots \\
\vdots & \vdots & \ddots & \ddots & 0 \\
0 & 0 & \ldots & 0 & 1 \\
1 & 0 & \ldots & 0 & 0
\end{pmatrix}. \tag{2.6}$$

The matrix P_N^n with $n \in \{-2, -3, \ldots\}$ is defined to be $(P_N^{-1})^{-n}$, which equals the transpose of P_N^{-n}, and the symbol $\otimes$ denotes the Kronecker product.

The matrix B_N has the form

$$B_N = \begin{pmatrix} W_1 & & W_2 \\ & \mathbf{0} & \\ W_3 & & W_4 \end{pmatrix}, \tag{2.7}$$

where W_1, W_2, W_3, and W_4 are $qw \times qw$ real matrices, $w \in \mathbb{Z}^+$; and w and W_j are constant and independent of N. B_N is defined for all $N \in \mathbb{Z}^+$ with $N > 2w$.

Similarly, $X_\alpha(q)$ is defined by setting $M_N = A_N$ in equality (2.3), and $X_\beta(q)$ by setting $M_N = B_N$.

Note that in the linear space $X(q)$, the subspace $X_r(q)$ is the sum of the linear subspaces $X_\alpha(q)$ and $X_\beta(q)$. One can equivalently define $X_r(q)$ to be the sum of these subspaces after defining them first.

We called $X_r(q)$, $X_\alpha(q)$, and $X_\beta(q)$, respectively, the repeat space, alpha space, and beta space with block-size q, and each element of $X_r(q)$, $X_\alpha(q)$, and $X_\beta(q)$, respectively, a repeat sequence, an alpha sequence, and a beta sequence with block-size q.

3. The Asymptotic Linearity Theorems that imply the Fukui conjecture

In this section, we chronologically review the ALTs from which the validity of the Fukui conjecture follows.

We need to recall some symbols used in the theorems.

Let M be an $n \times n$ Hermitian matrix and let φ be a real-valued function defined on a subset $S \subset \mathbb{R}$ such that the subset S contains all the eigenvalues of M. Let

$$M = \mu_1 P_{(1)} + \cdots + \mu_r P_{(r)} \tag{3.1}$$

be the spectral resolution of the Hermitian matrix M, where $\mu_1, \ldots, \mu_r$ are all the distinct eigenvalues of M and $P_{(1)}, \ldots, P_{(r)}$ are corresponding eigenprojections. Then, we define $\varphi(M)$ by

$$\varphi(M) = \varphi(\mu_1) P_{(1)} + \cdots + \varphi(\mu_r) P_{(r)}. \tag{3.2}$$

The fact that it is well defined is easily seen by the uniqueness of the spectral resolution.

Remark 3.1. (i) The matrix $\varphi(M)$ can be equivalently defined by

$$\varphi(M) = U \operatorname{diag}\big(\varphi(\lambda_1), \varphi(\lambda_2), \ldots, \varphi(\lambda_n)\big) U^{-1}, \tag{3.3}$$

where U is an $n \times n$ unitary matrix such that

$$U^{-1} M U = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n). \tag{3.4}$$

Note that

$$\operatorname{Tr} \varphi(M) = \operatorname{Tr}\big(U \operatorname{diag}\big(\varphi(\lambda_1), \varphi(\lambda_2), \ldots, \varphi(\lambda_n)\big) U^{-1}\big)$$

$$= \mathrm{Tr}\big(U^{-1}U\,\mathrm{diag}\big(\varphi(\lambda_1), \varphi(\lambda_2), \ldots, \varphi(\lambda_n)\big)\big)$$
$$= \sum_{i=1}^{n} \varphi(\lambda_i), \tag{3.5}$$

where Tr denotes the trace operation.

(ii) Let $I = [a, b]$ $(a, b \in \mathbb{R},\ a < b)$ denote a closed interval that contains all the eigenvalues of M. If $\varphi : I \to \mathbb{R}$ is a polynomial function with real coefficients defined by

$$\varphi(t) = c_0 t^0 + c_1 t^1 + \cdots + c_k t^k, \tag{3.6}$$

then the matrix $\varphi(M)$, defined by (3.2) or (3.3), is expressed by

$$\varphi(M) = c_0 M^0 + c_1 M^1 + \cdots + c_k M^k, \tag{3.7}$$

where M^0 denotes the $n \times n$ unit matrix.

Let $\{M_N\} \in X_r(q)$. A closed interval $I \subset \mathbb{R}$ is said to be *compatible with* $\{M_N\}$ if all the eigenvalues of M_N are contained in I for all $N \in \mathbb{Z}^+$. Given an $\{M_N\} \in X_r(q)$, the following proposition guarantees the existence of a closed interval I which is compatible with $\{M_N\} \in X_r(q)$.

Proposition 3.1. Let $\{M_N\} \in X_r(q)$. Let $\sigma(M_N)$ denote the set of all the eigenvalues of M_N. Then the union $\bigcup_{N \in \mathbb{Z}^+} \sigma(M_N)$ is a bounded set in $\mathbb{R}$.

Proof. This is easily verified by using a matrix norm [23,24] defined by $\|L\| = \max\{\sum_{j=1}^{n} |L_{ij}|\colon\ i \in \{1, 2, \ldots, n\}\}$ for an $n \times n$ matrix L. This norm gives an upper bound for the absolute values of the eigenvalues of L, i.e., if λ is an eigenvalue of L, then $|\lambda| \leqslant \|L\|$. Now, consider the real sequence $\{\|M_N\|\}$. Then paying attention to the repeating block pattern of M_N along the diagonal, we see immediately that $\|M_{N_0}\| = \|M_{N_0+1}\| = \cdots$ for some $N_0 \in \mathbb{Z}^+$. It clearly follows that $\bigcup_{N \in \mathbb{Z}^+} \sigma(M_N)$ is a bounded set in $\mathbb{R}$. □

Remark 3.2. (i) The boundedness of the union $\bigcup_{N \in \mathbb{Z}^+} \sigma(M_N)$ can be demonstrated in a broader context of the generalized repeat space; see [25, proposition 4.8].

(ii) Let $I = [a, b]$ $(a, b \in \mathbb{R}, a < b)$ denote a closed interval. A function $\varphi : I \to \mathbb{R}$ is said to be absolutely continuous on I if, given any $\varepsilon > 0$, there exists a $\delta > 0$ such that for every finite system of pairwise disjoint subintervals $(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n) \subset [a, b]$,

$$\sum_{k=1}^{n} (b_k - a_k) < \delta \tag{3.8}$$

implies

$$\sum_{k=1}^{n} \left|\varphi(b_k) - \varphi(a_k)\right| < \varepsilon. \tag{3.9}$$

(iii) If $\varphi : I \to \mathbb{R}$ is Lipschitz continuous, then φ is absolutely continuous on I.

(iv) If $\varphi : I \to \mathbb{R}$ is absolutely continuous, then φ is continuous and of bounded variation on I.

(v) It is easy to show that if ξ is a positive real number and $\varphi_\xi : I \to \mathbb{R}$ is defined by

$$\varphi_\xi(t) = |t|^\xi, \tag{3.10}$$

then φ_ξ is absolutely continuous on I.

Notation 3.1. Let $I = [a, b](a, b \in \mathbb{R}, a < b)$ denote a closed interval.

$V_I(\varphi)$: the total variation of a real-valued function φ on I, i.e.,

$$V_I(\varphi) = \sup_{\Delta} \sum_{i=1}^{n} \left|\varphi(t_i) - \varphi(t_{i-1})\right|, \tag{3.11}$$
$$\Delta:\ a = t_0 \leqslant t_1 \leqslant \cdots \leqslant t_n = b.$$

$BV(I)$: the set of all real-valued functions of bounded variation on I, i.e., the set of all real-valued functions φ on I such that $V_I(\varphi) < \infty$.

$CBV(I)$: the normed space of all real-valued continuous functions of bounded variation on I equipped with the norm given by

$$\|\varphi\| = \sup\left\{\left|\varphi(t)\right|:\ t \in I\right\} + V_I(\varphi). \tag{3.12}$$

$AC(I)$: the normed space of all real-valued absolutely continuous functions on I equipped with the norm given by

$$\|\varphi\| = \sup\left\{\left|\varphi(t)\right|:\ t \in I\right\} + V_I(\varphi). \tag{3.13}$$

$P(I)$: the set of all polynomial functions with real coefficients defined on I.

$\overline{}$: the closure operation on a topological space.

$\boldsymbol{B}(X, Y)$: the normed space of all bounded linear operators from a normed space X to a normed space Y.

$CBV(I)^*$: the dual space of $CBV(I)$, i.e.,

$$CBV(I)^* = \boldsymbol{B}\big(CBV(I), \mathbb{R}\big). \tag{3.14}$$

$AC(I)^*$: the dual space of $AC(I)$, i.e.,

$$AC(I)^* = \boldsymbol{B}\big(AC(I), \mathbb{R}\big). \tag{3.15}$$

We retain the above notation 3.1 throughout this article. We remark that if E denotes a normed space, we also let E stand for the underlying set of the normed space when no confusion arises. The following proposition has been of fundamental importance in the development and applications of the ALTs.

Proposition 3.2. The notation being as above, the closure of $P(I)$ in the normed space $CBV(I)$ coincides with the underlying set of the normed space $AC(I)$, in symbol,

$$AC(I) = \overline{P(I)} \subset CBV(I). \tag{3.16}$$

Proof. See [26] for a detailed proof of the proposition (also for the applications of theorem 3.3 to thermodynamic additivity problems). □

Note that $AC(I)$ forms a subspace of the normed space $CBV(I)$.

Recall that a real sequence E_N is said to have an asymptotic line if there exist α, $\beta \in \mathbb{R}$ such that $E_N - (\alpha N + \beta) \to 0$ as $N \to \infty$, i.e., if there exist $\alpha, \beta \in \mathbb{R}$ such that $E_N = \alpha N + \beta + o(1)$, as $N \to \infty$, where $o(1)$ denotes the Landau notation.

Now we are ready to chronologically review the ALTs from which the validity of the Fukui conjecture follows.

Theorem 3.1 (Original ALT, $X_r(q)$-version and the "$\varphi_{1/2}$-proposition": (ii)). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then we have

(i) For any $\varphi \in \overline{P(I)} \subset CBV(I)$, $\mathrm{Tr}\,\varphi(M_N)$ has an asymptotic line.

(ii) $\varphi_{1/2} \in \overline{P(I)} \subset CBV(I)$, where $\varphi_{1/2}(t) = |t|^{1/2}$.

Proof. The first proof of this theorem was given in [27, chapter 7] according to the method and outline of the proof described in [22]. (Let ξ be any positive real number, define $\varphi_\xi : I \to \mathbb{R}$ by (3.10), the relation $\varphi_\xi \in \overline{P(I)} \subset CBV(I)$ was also proved in [27, chapter 7].) □

Theorem 3.2 (Original ALT, $X_r(q)$-version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in \overline{P(I)} \subset CBV(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\mathrm{Tr}\,\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{3.17}$$

as $N \to \infty$.

Proof. A proof using diagrams of arrows was given in [28]. (The method using diagrams of arrows has played an important part in the RST, and this method originates in [28]. Cf. also remark 4.1 in section 4.) □

Theorem 3.3 (Practical ALT, $X_r(q)$-version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in AC(I)$, there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{3.18}$$

as $N \to \infty$.

Proof. The conclusion immediately follows from theorem 3.1 (or theorem 3.2) together with proposition 3.2 (cf. [26]). □

Theorem 3.4 (Functional ALT, $X_r(q)$-version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, there exist functionals $\alpha, \beta \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{3.19}$$

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

Theorem 3.1, which explicitly shows that the Fukui conjecture is true, was first proved in [27, chapter 7]. The generic name “Asymptotic Linearity Theorem” originates in theorem 3.1, which contains the words “asymptotic line” in its assertion.

Once $\varphi_{1/2} \in \overline{P(I)} \subset CBV(I)$ was established and the extensiveness of the $\overline{P(I)}$ was recognized, the “$\varphi_{1/2}$-proposition” began to be omitted in the subsequent versions of Asymptotic Linearity Theorems.

We may now summarize the relationship between theorems 3.1, 3.2, and 3.3, as follows:

- theorem 3.1 $\Rightarrow$ theorem 3.2.
- theorem 3.2 and proposition 3.2 $\Rightarrow$ theorem 3.3.

We may also summarize the relationship between the Functional ALT, theorems 3.1–3.3, and the validity of the Fukui conjecture, as follows:

- Functional ALT (theorem 3.4) $\Rightarrow$ theorems 3.1, 3.2 and 3.3 $\Rightarrow$ the Fukui conjecture.

Remark 3.3. The author is indebted to Professors M. Spivakovsky, K. Saito and I. Naruki, who provided him with an important lemma (Piecewise Monotone Lemma) which has been indispensable for establishing any version of the ALTs that imply the Fukui conjecture.

4. Formulation of a problem and fundamental theorems for the proof of the Functional Asymptotic Linearity Theorem

We begin this section by formulating a problem whose affirmative solution given in section 6 will streamline our argument in handling key inequalities essential for establishing any version of the ALTs that can prove the Fukui conjecture.

Let $\{M_N\} \in X_r(q)$ and let I be a closed interval compatible with $\{M_N\}$. Let $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$ be such that

$$\{M_N\} = \{A_N\} + \{B_N\}. \tag{4.1}$$

Let J be a closed interval which contains I and is compatible with both $\{M_N\}$ and $\{A_N\}$. By considering two such intervals I and J and the associated functional spaces $CBV(I)$ and $CBV(J)$, we could define the quantities $\varphi(M_N)$ and $\varphi(A_N)$ with $\varphi \in CBV(J)$ and could obtain key inequalities for the proof of the Original ALT. However, if the following problem is affirmatively solved, the proofs of both the Original and Functional ALTs can be simplified.

Problem I. Let $\{M_N\} \in X_r(q)$. By suitably selecting $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$ under the condition (4.1), can we dispense with the extended interval J and its associated functional space $CBV(J)$ so that we can only consider I and $CBV(I)$? In other words, is the following statement true?

Statement I. Let $\{M_N\} \in X_r(q)$ and let I be a closed interval compatible with $\{M_N\}$. Then there exist $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$ such that $\{M_N\} = \{A_N\} + \{B_N\}$ and such that I is also compatible with $\{A_N\}$.

We remark that statement I is true. In the end of section 6, we shall prove statement I using what we call the Compatibility Theorem (theorem 6.1), whose proof is given in section 7. In section 5, we provide a proof of the Functional ALT assuming the validity of statement I. (We note that only the reader who is familiar with the compatibility problem should read sections 6 and 7 first before reading section 5.)

In what follows, we recall the Polynomial ALT (theorem 4.1) from [22,28] and its logical precursor: theorem 4.2 from [22]. We also establish a topological closure extension theorem, theorems 4.3 and its logical precursor: theorem 4.4. These four theorems (theorems 4.1–4.4) are of fundamental significance for proving and gaining a logical insight into the assertion of our main theorem, the Functional ALT.

Remark 4.1. The reader is referred to [1,22,28] for the following two complementary unifying approaches:

(i) the approach via the aspect of form,

(ii) the approach via the aspect of general topology, which originate in [22] and have played a central role in the RST to systematically obtain solutions for a variety of additivity and network problems. We remark that theorems 4.1 and 4.2 correspond to (i) and theorems 4.3 and 4.4 correspond to (ii). We also remark that in the recent development of the RST, "the approach using diagrams of arrows", which originates in [28] has been incorporated into (ii).

Theorem 4.1 (Polynomial ALT, $X_r(q)$-version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence. Let I be a fixed closed interval compatible with $\{M_N\}$. Then, for any $\varphi \in P(I)$ there exist $\alpha(\varphi), \beta(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) \tag{4.2}$$

for all $N \gg 0$.

Proof. The conclusion immediately follows from the definition of $X_r(q)$ and the following theorem 4.2 (cf. also [22,28]). □

Theorem 4.2. Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence. Let I be a fixed closed interval compatible with $\{M_N\}$. Suppose that $\varphi \in P(I)$, then we have

$$\bigl\{\varphi(M_N)\bigr\} \in X_r(q). \tag{4.3}$$

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

$$\varphi(t) = c_0 t^0 + \cdots + c_n t^n, \tag{4.4}$$

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

$$\bigl\{\varphi(M_N)\bigr\} = \bigl\{c_0 M_N^0 + \cdots + c_n M_N^n\bigr\} \tag{4.5}$$

and that

$$\bigl\{M_N^0\bigr\} = \{qN \times qN \text{ unit matrix}\} \in X_r(q). \tag{4.6}$$

Since $X_r(q)$ is a linear space, to show that (4.3) is true, we have only to verify that

$$\bigl\{M_N^m\bigr\} \in X_r(q) \tag{4.7}$$

for each $m \in \mathbb{Z}^+$. But, (4.7) can be easily proved by induction on m, bearing in mind the fact that $X_r(q)$ is closed under the Jordan product operation $\circ$ defined by

$$\{K_N\} \circ \{L_N\} = \bigl\{\tfrac{1}{2}(K_N L_N + L_N K_N)\bigr\}. \tag{4.8}$$

(cf. [22] for details). □

Theorem 4.3. Let $\mathbb{K}$ denote either the real field $\mathbb{R}$, or the complex field $\mathbb{C}$. Let X be a normed space over $\mathbb{K}$, let $\mathscr{B}$ be a Banach space over $\mathbb{K}$, and let $\tau_N \in \boldsymbol{B}(X, \mathscr{B})$ be a sequence of bounded linear operators from X to $\mathscr{B}$. Let $\boldsymbol{L}$ denote the topological space with the underlying set $\{\boldsymbol{T}, \boldsymbol{F}\}$ and the system of open sets $o_{\boldsymbol{T}} = \{\varnothing, \{\boldsymbol{F}\}, \{\boldsymbol{T}, \boldsymbol{F}\}\}$. Consider the mapping $\pi : X \to \boldsymbol{L}$ defined by

$$\pi(\varphi) = \begin{cases} \boldsymbol{T} & \text{if } \{\tau_N(\varphi)\} \text{ is convergent,} \\ \boldsymbol{F} & \text{if } \{\tau_N(\varphi)\} \text{ is not convergent.} \end{cases} \tag{4.9}$$

Suppose that

$$\sup\bigl\{\|\tau_N\|:\ N \geqslant 1\bigr\} < \infty. \tag{4.10}$$

Then, the following statements are true:

(i) π is continuous.

(ii) If X_0 is a subset of X with $\pi(X_0) = \{\boldsymbol{T}\}$, then $\pi(\overline{X_0}) = \{\boldsymbol{T}\}$.

(iii) If X_0 is a dense subset of X with $\pi(X_0) = \{\boldsymbol{T}\}$, then $\pi(X) = \{\boldsymbol{T}\}$, moreover, $\tau : X \to \mathscr{B}$ defined by $\tau(\varphi) = \lim_{N\to\infty} \tau_N(\varphi)$ is a bounded linear operator: $\tau \in \boldsymbol{B}(X, \mathscr{B})$.

Proof. (i) Under the assumptions of the theorem, consider the mapping $\pi_0 : X \to \boldsymbol{L}$ defined by

$$\pi_0(\varphi) = \begin{cases} \boldsymbol{T} & \text{if } \{\tau_N(\varphi)\} \text{ is a Cauchy sequence,} \\ \boldsymbol{F} & \text{if } \{\tau_N(\varphi)\} \text{ is not a Cauchy sequence.} \end{cases} \tag{4.11}$$

Then, because $\mathscr{B}$ is complete, we see that

$$\pi = \pi_0. \tag{4.12}$$

But, theorem 4.4 below implies that π_0 is continuous. Hence, π is continuous.

(ii) Suppose that X_0 is a subset of X with $\pi(X_0) = \{\boldsymbol{T}\}$. Then by (i), we have $\pi(\overline{X_0}) \subset \overline{\pi(X_0)}$. This implies that $\pi(\overline{X_0}) \subset \{\boldsymbol{T}\}$. The opposite inclusion $\pi(\overline{X_0}) \supset \{\boldsymbol{T}\}$ is obvious.

(iii) By (ii), it remains to prove that the operator τ is linear and bounded. Since τ_N is linear, the linearity of τ is obvious. The boundedness follows from the relations:

$$\begin{aligned} \|\tau(\varphi)\| &= \Bigl\| \lim_{N\to\infty} \tau_N(\varphi) \Bigr\| \\ &= \lim_{N\to\infty} \|\tau_N(\varphi)\| \\ &= \varliminf_{N\to\infty} \|\tau_N(\varphi)\| \\ &\leqslant \Bigl(\varliminf_{N\to\infty} \|\tau_N\| \Bigr) \|\varphi\| \\ &\leqslant \bigl(\sup\bigl\{\|\tau_N\|:\ N \geqslant 1\bigr\}\bigr) \|\varphi\|. \end{aligned} \tag{4.13}$$

□

Theorem 4.4. Let $\mathbb{K}$ denote either the real field $\mathbb{R}$, or the complex field $\mathbb{C}$. Let X and Y be normed spaces over $\mathbb{K}$ and let $\tau_N \in \boldsymbol{B}(X, Y)$ be a sequence of bounded linear operators from X to Y. Let Y^∞ denote the normed space of all the sequences $\{a_N\}$ in Y with $\sup\{\|a_N\|: N \geqslant 1\} < \infty$, equipped with the norm given by

$$\big\|\{a_N\}\big\| = \sup\big\{\|a_N\|: N \geqslant 1\big\}, \tag{4.14}$$

and let $\boldsymbol{L}$ denote the topological space with the underlying set $\{\boldsymbol{T}, \boldsymbol{F}\}$ and the system of open sets $o_{\boldsymbol{T}} = \{\varnothing, \{\boldsymbol{F}\}, \{\boldsymbol{T}, \boldsymbol{F}\}\}$. Let $\pi_0 : X \to \boldsymbol{L}$ be a mapping such that the following diagram is commutative:

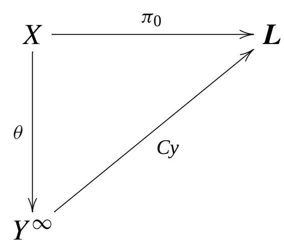

Diagram I.

That is, let

$$\pi_0 = Cy \circ \theta. \tag{4.15}$$

Here, θ and Cy are defined by

$$\theta(\varphi) = \big\{\tau_N(\varphi)\big\}, \tag{4.16}$$

$$Cy\big(\{a_N\}\big) = \begin{cases} \boldsymbol{T} & \text{if } \{a_N\} \text{ is a Cauchy sequence,} \\ \boldsymbol{F} & \text{if } \{a_N\} \text{ is not a Cauchy sequence.} \end{cases} \tag{4.17}$$

Suppose that

$$\sup\big\{\|\tau_N\|: N \geqslant 1\big\} < \infty. \tag{4.18}$$

Then, π_0 is continuous.

Proof. We first show that θ is continuous. It is easy to see that θ is linear. Hence, it suffices to verify that θ is bounded. Assume that $\sup\{\|\tau_N\|: N \geqslant 1\} < \infty$, and let $\varphi \in X$. Then we have

$$\begin{aligned} \|\theta(\varphi)\| &= \big\|\big\{\tau_N(\varphi)\big\}\big\| \\ &= \sup\big\{\big\|\tau_N(\varphi)\big\|: N \geqslant 1\big\} \\ &\leqslant \big(\sup\big\{\|\tau_N\|: N \geqslant 1\big\}\big)\|\varphi\|, \end{aligned} \tag{4.19}$$

which shows that θ is bounded.

Second, we verify that the mapping Cy is continuous. Consider the following diagram II, where θ' and θ'' are defined by

$$\theta'\big(\{a_n\}\big) = \lim_{N_0 \to \infty} \sup\big\{\|a_m - a_n\|: m, n \geqslant N_0\big\}, \tag{4.20}$$

$$\theta''(x) = \begin{cases} \boldsymbol{T} & \text{if } x = 0, \\ \boldsymbol{F} & \text{if } x \neq 0. \end{cases} \tag{4.21}$$

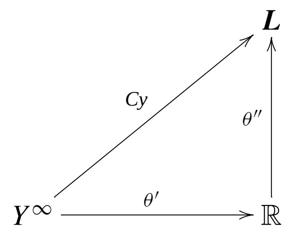

Diagram II.

Note first that diagram II is commutative and θ'' is clearly continuous. Thus, to verify that Cy is continuous, it suffices to show that θ' is continuous. The continuity of θ' easily follows from the fact that θ' is a semi-norm on the linear space Y^∞, i.e., θ' is a real-valued mapping on Y^∞ which satisfies the following relations for all $a, b \in Y^\infty$ and $k \in \mathbb{K}$:

$$\theta'(a) \geqslant 0, \tag{4.22}$$

$$\theta'(ka) = |k|\theta'(a), \tag{4.23}$$

$$\theta'(a+b) \leqslant \theta'(a) + \theta'(b). \tag{4.24}$$

From this, we easily have for all $a, b \in Y^\infty$

$$\left|\theta'(a) - \theta'(b)\right| \leqslant \theta'(a-b), \tag{4.25}$$

and hence

$$\left|\theta'(a) - \theta'(b)\right| \leqslant 2\|a-b\| \tag{4.26}$$

which implies that θ' is Lipschitz continuous and thus continuous. Now the continuity of Cy has been proved.

By (4.15), $\pi_0 = Cy \circ \theta$, and we have verified that both θ and Cy are continuous. Therefore, π_0 is continuous. □

Remark 4.2. We remark that theorems 4.3 and 4.4 and their proofs can be used to gain a deeper insight into lemma 3.2 and the topological closure extension procedures given in [29], and that theorems 4.3 and 4.4 here established can be applied to similar extension procedures given in [25,29–31].

The rest of this section is devoted to establishing theorem 4.5 by using theorems 4.1 and 4.3. We note that theorem 4.5 is used to formulate theorem 5.1 in section 5 (cf. remark 5.1). The reader is referred to [32] for the original form of theorem 4.5, and also to [25,29–31] for generalizations of theorem 4.5.

Notation 4.1. Let $I = [a, b]$ $(a, b \in \mathbb{R},\ a < b)$ denote a closed interval.

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

$$\|\varphi\|_{\mathrm{u}} = \sup\bigl\{\bigl|\varphi(t)\bigr|\colon\ t \in I\bigr\}. \tag{4.27}$$

$C(I)^*$: the dual space of $C(I)$, i.e.,

$$C(I)^* = \boldsymbol{B}\bigl(C(I), \mathbb{R}\bigr). \tag{4.28}$$

Theorem 4.5 (Functional Alpha Existence Theorem, $X_r(q)$ version). Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let I be a fixed closed interval compatible with $\{M_N\}$. Then, there exists a functional $\alpha \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ such that

$$\frac{\operatorname{Tr}\varphi(M_N)}{N} = \alpha(\varphi) + o(1) \tag{4.29}$$

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

Proof. Define the sequence of linear functionals $\alpha_N \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$ by

$$\alpha_N(\varphi) = \frac{\operatorname{Tr}\varphi(M_N)}{N}. \tag{4.30}$$

Recall the Stone–Weierstrass theorem, which implies that $P(I)$ is a dense subset of $C(I)$:

$$\overline{P(I)} = C(I). \tag{4.31}$$

It is easy to check that

(A1) for all $\varphi \in P(I)$, $\lim_{N\to\infty} \alpha_N(\varphi)$ exists in $\mathbb{R}$,

(A2) $\sup\{\|\alpha_N\|\colon\ N \geqslant 1\} < \infty$,

(A3) for all $\varphi \in C(I)$, $\lim_{N\to\infty} \alpha_N(\varphi)$ exists in $\mathbb{R}$,

(A4) $\alpha : C(I) \to \mathbb{R}$ defined by

$$\alpha(\varphi) = \lim_{N\to\infty} \alpha_N(\varphi) \tag{4.32}$$

is a bounded linear functional: $\alpha \in C(I)^* = \boldsymbol{B}(C(I), \mathbb{R})$.

In fact, (A1) follows from theorem 4.1, (A2) from the easily verifiable relations

$$\bigl|\alpha_N(\varphi)\bigr| \leqslant q\bigl(\sup\bigl\{\bigl|\varphi(t)\bigr|\colon\ t \in I\bigr\}\bigr) = q\|\varphi\|_{\mathrm{u}} \tag{4.33}$$

valid for all $\varphi \in C(I)$ and $N \in \mathbb{Z}^+$. Note that (4.31), (A1), (A2), and theorem 4.3(iii) imply (A3) and (A4). From (A4) the conclusion follows. □

We recall remark 4.1 and note that the above proof of theorem 4.5 (Functional AET) has been made by using (i) the approach via the aspect of form (in conjunction with theorems 4.1 and 4.2) and (ii) the approach via the aspect of general topology (in conjunction with theorems 4.3 and 4.4). The above proof of the Functional AET using unifying approaches (i) and (ii) is prototypical for the proofs of diverse existence theorems in the RST. The insights it provides are crucial for understanding the next section.

In section 5, we shall use this prototype as a guideline for establishing our main theorem, the Functional ALT.

5. Proof of the Functional Asymptotic Linearity Theorem

There are a number of ways of proving the Functional ALT with varying degrees of dependence on the original ALT. Here, we shall prove this theorem without using the Original ALT.

Before proving the Functional ALT, we need some preparation.

Theorem 5.1. Let $\{M_N\} \in X_r(q)$ and let I be a closed interval compatible with $\{M_N\}$. Given $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$ such that

$$\{M_N\} = \{A_N\} + \{B_N\}, \tag{5.1}$$

let J be a closed interval which contains I and is compatible with both $\{M_N\}$ and $\{A_N\}$.

Define the sequence of functionals $\beta_N^I \in CBV(I)^* = \boldsymbol{B}(CBV(I), \mathbb{R})$ by

$$\beta_N^I(\varphi) = \operatorname{Tr}\varphi(M_N) - \alpha^I(\varphi)N, \tag{5.2}$$

where

$$\alpha^I(\varphi) := \lim_{N\to\infty} \frac{\operatorname{Tr}\varphi(M_N)}{N}. \tag{5.3}$$

Similarly, define the sequence of functionals $\beta_N^J \in CBV(J)^* = \boldsymbol{B}(CBV(J), \mathbb{R})$ by

$$\beta_N^J(\varphi) = \operatorname{Tr}\varphi(M_N) - \alpha^J(\varphi)N, \tag{5.4}$$

where

$$\alpha^J(\varphi) := \lim_{N\to\infty} \frac{\operatorname{Tr}\varphi(M_N)}{N}. \tag{5.5}$$

Let $\beta_N^{(I)}$ denote the restriction of β_N^I to the subspace $AC(I)$ of the normed space $CBV(I)$:

$$\beta_N^{(I)} = \beta_N^I\big|_{AC(I)}. \tag{5.6}$$

Then, we have

$$\text{(i)} \quad \sup\left\{\left\|\beta_N^J\right\|:\ N \geqslant 1\right\} < \infty, \tag{5.7}$$

$$\text{(ii)} \quad \sup\left\{\left\|\beta_N^I\right\|:\ N \geqslant 1\right\} < \infty, \tag{5.8}$$

$$\text{(iii)} \quad \sup\left\{\left\|\beta_N^{(I)}\right\|:\ N \geqslant 1\right\} < \infty. \tag{5.9}$$

Remark 5.1. (i) To see that the above $\alpha^I(\varphi)$ and $\alpha^J(\varphi)$ are well defined, recall theorem 4.5 and notice that $CBV(I) \subset C(I)$.

(ii) To see that $\beta_N^I \in CBV(I)^*$, note that the following relations:

$$\begin{aligned} |\beta_N^I(\varphi)| &\leqslant \left|\operatorname{Tr}\varphi\bigl(M_N\bigr)\right| + \left|\alpha^I(\varphi)N\right| \\ &\leqslant 2qN\bigl(\sup\bigl\{\left|\varphi(t)\right|:\ t \in I\bigr\}\bigr) \\ &\leqslant 2qN\bigl(\sup\bigl\{\left|\varphi(t)\right|:\ t \in I\bigr\} + V_I(\varphi)\bigr) = 2qN\|\varphi\| \end{aligned} \tag{5.10}$$

hold for all $\varphi \in CBV(I)$ and $N \in \mathbb{Z}^+$. Hence, $\beta_N^I \in CBV(I)^*$, and similarly we have $\beta_N^J \in CBV(J)^*$ for all $N \in \mathbb{Z}^+$.

Proof of theorem 5.1. (i) This immediately follows from inequality (13) in [27, chapter 7, p. 198]. (We remark that this is also an immediate consequence of proposition ES# in [28, p. 230].)

(ii) We recall statement I, which was given in section 4 and is going to be proved in section 6 via the Compatibility Theorem. Notice that statement I implies that there exist $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$ such that (5.1) is true and such that interval I is also compatible with $\{A_N\}$. Consider such special $\{A_N\} \in X_\alpha(q)$ and $\{B_N\} \in X_\beta(q)$, and set $J = I$ in (i) to obtain (ii).

(iii) It is easy to see that $\|\beta_N^{(I)}\| \leqslant \|\beta_N^I\|$ for all $N \in \mathbb{Z}^+$, which obviously implies that (iii) is true. □

Once the Compatibility Theorem is established and we see that statement I is true, consideration on the extended interval J and its associated functional space $CBV(J)$ become unnecessary. However, the following proof of theorem 5.1, part (ii), is instructive to understand one of the methods to overcome the "compatibility problem" in the proofs of the Original and Functional ALTs.

The second proof of theorem 5.1(ii). Consider the mapping $T : CBV(I) \to CBV(J)$ defined by

$$T(\varphi)(x) = \begin{cases} \varphi(a) & \text{if } x \in [A, a), \\ \varphi(x) & \text{if } x \in [a, b], \\ \varphi(b) & \text{if } x \in (b, B], \end{cases} \tag{5.11}$$

where $I = [a, b]$, $J = [A, B]$, $A \leqslant a < b \leqslant B$. It is easily verified that T is linear and bounded satisfying the relation

$$\left\|T(\varphi)\right\| = \|\varphi\| \tag{5.12}$$

for all $\varphi \in CBV(I)$. Note that

$$\beta_N^I = \beta_N^J \circ T, \tag{5.13}$$

and that

$$\left|\beta_N^I(\varphi)\right| \leqslant \left\|\beta_N^J\right\|\left\|T(\varphi)\right\| = \left\|\beta_N^J\right\|\left\|\varphi\right\|, \tag{5.14}$$

for all $\varphi \in CBV(I)$. Hence, we have

$$\|\beta_N^I\| \leqslant \|\beta_N^J\|, \tag{5.15}$$

which together with (i) implies (ii). □

We are now ready to give a proof of the Functional ALT.

Proof of the Functional ALT. Define the sequence of linear functionals $\alpha_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ by

$$\alpha_N(\varphi) = \frac{\operatorname{Tr}\varphi(M_N)}{N}. \tag{5.16}$$

Recall the fact that $P(I)$ is a dense subset of $AC(I)$:

$$\overline{P(I)} = AC(I) \tag{5.17}$$

(cf. proposition 3.2).

It is easy to check that

(a1) for all $\varphi \in P(I)$, $\lim_{N\to\infty} \alpha_N(\varphi)$ exists in $\mathbb{R}$,

(a2) $\sup\{\|\alpha_N\|: N \geqslant 1\} < \infty$,

(a3) for all $\varphi \in AC(I)$, $\lim_{N\to\infty} \alpha_N(\varphi)$ exists in $\mathbb{R}$,

(a4) $\alpha : AC(I) \to \mathbb{R}$ defined by

$$\alpha(\varphi) = \lim_{N\to\infty} \alpha_N(\varphi) \tag{5.18}$$

is a bounded linear functional: $\alpha \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$.

In fact, statement (a1) follows from theorem 4.1 and statement (a2) follows from the easily verifiable relations

$$\begin{aligned} \left|\alpha_N(\varphi)\right| &\leqslant q\left(\sup\left\{\left|\varphi(t)\right|: t \in I\right\}\right) \\ &\leqslant q\left(\sup\left\{\left|\varphi(t)\right|: t \in I\right\} + V_I(\varphi)\right) = q\|\varphi\| \end{aligned} \tag{5.19}$$

valid for all $\varphi \in AC(I)$ and $N \in \mathbb{Z}^+$. Note that (5.17), (a1), (a2), and theorem 4.3(iii) imply (a3) and (a4).

Using equality (5.18), define the sequence of linear functionals $\beta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ by

$$\beta_N(\varphi) = \operatorname{Tr}\varphi(M_N) - \alpha(\varphi)N. \tag{5.20}$$

We now verify that

(b1) for all $\varphi \in P(I)$, $\lim_{N\to\infty} \beta_N(\varphi)$ exists in $\mathbb{R}$,

(b2) $\sup\{\|\beta_N\|: N \geqslant 1\} < \infty$,

(b3) for all $\varphi \in AC(I)$, $\lim_{N\to\infty} \beta_N(\varphi)$ exists in $\mathbb{R}$, (b4) $\beta : AC(I) \to \mathbb{R}$ defined by

$$\beta(\varphi) = \lim_{N\to\infty} \beta_N(\varphi) \tag{5.21}$$

is a bounded linear functional: $\beta \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$.

It is easily seen that (b1) follows from theorem 4.1 and that (b2) follows from theorem 5.1(iii). Note that (5.17), (b1), (b2), and theorem 4.3(iii) imply (b3) and (b4).

From (a4) and (b4) the conclusion of the theorem follows. □

6. Notion of the standard alpha space $X_{\#\alpha}(q)$ and other preliminaries for the Compatibility Theorem

We begin this section by recalling a couple of notions from [20], which are summarized in definitions 6.1 and form a basis for what follows.

Definitions 6.1. Fix a $q \in \mathbb{Z}^+$, and let $h(q)$ denote the linear space over the field $\mathbb{R}$ of all $q \times q$ Hermitian matrices, and let $H(q)$ denote the set of all mappings $F : \mathbb{R} \to h(q)$, i.e., the set of all $q \times q$ Hermitian-matrix-valued functions defined on the real line. Let $H_f(q) \subset H(q)$ denote the subset of all mappings F that have the form of a finite Fourier series:

$$F(\theta) = \sum_{n=-\nu}^{\nu} \big(\exp(\mathrm{i}n\theta)\big) Q_n, \quad Q_{-n} = Q_n^{\mathrm{T}}, \qquad n = 0, 1, \ldots, \nu, \tag{6.1}$$

$\theta \in \mathbb{R}$, where ν is a nonnegative integer, $Q_0, Q_1, \ldots, Q_\nu$ are all $q \times q$ real matrices and Q_n^{T} denotes the transpose of Q_n.

Define $\Omega : X_r(q) \to H_f(q)$ by the following procedure. Given any $\{M_N\} \in X_r(q)$, then by the definition of the repeat space, there is a pair of sequences $\{A_N\} \in X_\alpha(q)$, $\{B_N\} \in X_\beta(q)$ whose sum equals $\{M_N\}$, and a nonnegative integer ν and matrices $Q_{-\nu}, Q_{-\nu+1}, \ldots, Q_\nu$ as in (2.4) and (2.5) such that for all $N \gg 0$ the Nth term M_N of $\{M_N\}$ is expressed as

$$M_N = A_N + B_N = \sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n + B_N. \tag{6.2}$$

The mapping Ω is then defined by

$$\Omega\big(\{M_N\}\big)(\theta) = \sum_{n=-\nu}^{\nu} \big(\exp(\mathrm{i}n\theta)\big) Q_n. \tag{6.3}$$

It is not difficult to see that this mapping is well defined (cf. [20] for detailed discussion on the mapping Ω, cf. also remark 6.1 given later in this section).

Given any $\{M_N\} \in X_r(q)$, we called $F = \Omega(\{M_N\}) \in H_f(q)$ the FS *map associated with the repeat sequence* $\{M_N\}$. A closed interval $I \subset \mathbb{R}$ was said to be *compatible* *with* F if I contains all the eigenvalues of $F(\theta)$ for all $\theta \in \mathbb{R}$. The existence of such an interval for any $F \in H_f(q)$ will be clear in view of proposition 6.2(i) given below and of the fact that F is a periodic mapping with the period 2π, that is $F(\theta) = F(\theta + 2\pi)$ for all $\theta \in \mathbb{R}$ (cf. also [20]).

In what follows, we provide the definitions of a standard alpha sequence with block-size q, and the standard alpha space with block-size q denoted by $X_{\#\alpha}(q)$, which are important ingredients in the Compatibility Theorem given at the end of this section.

Definitions 6.2. Let $q \in \mathbb{Z}^+$. An alpha sequence $\{A_N\} \in X_\alpha(q)$ is called a *standard alpha sequence* with block-size q, or a *standard element of* $X_\alpha(q)$, if there exist a non-negative integer ν and $q \times q$ real matrices $Q_{-\nu}, Q_{-\nu+1}, \ldots, Q_\nu$ such that

$$A_N = \sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n \tag{6.4}$$

for all $N \in \mathbb{Z}^+$. (Note that Q_{-n} is the transpose of Q_n for all $n \in \{0, 1, \ldots, \nu\}$ since $X_\alpha(q) \subset X(q)$.)

For each $q \in \mathbb{Z}^+$, let $X_{\#\alpha}(q)$ denote the set of all standard elements of $X_\alpha(q)$. The $X_{\#\alpha}(q)$ is called the *standard alpha space* with block-size q.

The following proposition illuminates the relationship between, $X_r(q)$, $X_{\#\alpha}(q)$, $X_\alpha(q)$, and $X_\beta(q)$, and is also helpful to see the structure of the mapping Ω defined above (cf. remark 6.1).

Proposition 6.1. For each $q \in \mathbb{Z}^+$, we have

(i) $X_{\#\alpha}(q)$ forms a linear subspace of $X_\alpha(q)$ and of $X_r(q)$.

(ii) $X_r(q)$ is the direct sum of its linear subspaces $X_{\#\alpha}(q)$ and $X_\beta(q)$:

$$X_r(q) = X_{\#\alpha}(q) \dot{+} X_\beta(q). \tag{6.5}$$

Proof. (i) The conclusion easily follows from the definitions of $X_{\#\alpha}(q)$, $X_\alpha(q)$, and $X_r(q)$.

(ii) Note that

$$X_r(q) = \operatorname{span}\big(X_{\#\alpha}(q) \cup X_\beta(q)\big), \tag{6.6}$$

where span denotes the linear span. We see that (ii) is true since $X_{\#\alpha}(q) \cap X_\beta(q)$ consists of a single repeat sequence whose Nth term is $qN \times qN$ zero matrix. □

Remark 6.1. Proposition 6.1(ii) implies that any element $\{M_N\}$ of $X_r(q)$ is expressed uniquely as the sum of $\{A_N\} \in X_{\#\alpha}(q)$ and $\{B_N\} \in X_\beta(q)$. Let $\mathrm{pr}_1 : X_r(q) \to X_{\#\alpha}(q)$

denote the first projection, $\mathrm{pr}_1(\{M_N\}) = \{A_N\}$. Let $\Omega_0 : X_{\#\alpha}(q) \to H_f(q)$ denote the mapping defined by

$$\Omega_0\left(\left\{\sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n\right\}\right)(\theta) = \sum_{n=-\nu}^{\nu} \bigl(\exp(\mathrm{i}n\theta)\bigr) Q_n. \tag{6.7}$$

Then, the mapping $\Omega : X_r(q) \to H_f(q)$ defined previously is expressed in terms of Ω_0 and pr_1:

$$\Omega = \Omega_0 \circ \mathrm{pr}_1. \tag{6.8}$$

The following proposition is going to be used in the Compatibility Theorem.

Proposition 6.2. Suppose that $\{A_N\} \in X_{\#\alpha}(q)$ and that A_N is given by

$$A_N = \sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n, \tag{6.9}$$

for all $N \in \mathbb{Z}^+$, where ν is a nonnegative integer and $Q_{-\nu}, Q_{-\nu+1}, \ldots, Q_\nu$ are $q \times q$ real matrices such that Q_{-n} is the transpose of Q_n for all $n \in \{0, 1, \ldots, \nu\}$. Let F be the FS-map associated with the $\{A_N\}$, i.e., let $F \in H_f(q)$ be a mapping defined by

$$F(\theta) = \sum_{n=-\nu}^{\nu} \bigl(\exp(\mathrm{i}n\theta)\bigr) Q_n, \tag{6.10}$$

$\theta \in \mathbb{R}$. Define functions $h_j : \mathbb{R} \to \mathbb{R}$, $j \in \{1, \ldots, q\}$ by

$$h_j(\theta) = \lambda_j(F(\theta)), \tag{6.11}$$

where $\lambda_j(F(\theta))$ denotes the jth eigenvalue of the Hermitian matrix $F(\theta)$ counting the multiplicity, arranged in the increasing order. Then, we have:

(i) h_j is Lipschitz continuous for all $j \in \{1, \ldots, q\}$.

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

$$(U_N \otimes I_q)^{-1} A_N (U_N \otimes I_q) = \text{B-diag}\left(F\left(\frac{2\pi}{N}\right), F\left(\frac{2\pi 2}{N}\right), \ldots, F\left(\frac{2\pi N}{N}\right)\right), \tag{6.12}$$

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

$$(U_N)_{mn} = N^{-1/2} \exp\left(\frac{2\pi mn\mathrm{i}}{N}\right), \tag{6.13}$$

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

Proof. Both (i) and (ii) were proved in [20]. We reproduce here only the proof of (ii).

By using the fundamental properties of the Kronecker product and the elementary equality for the diagonalization of P_N:

$$U_N^{-1} P_N U_N = \operatorname{diag}\left(\exp\left(\frac{2\pi \mathrm{i}}{N}\right), \exp\left(\frac{2\pi 2\mathrm{i}}{N}\right), \dots, \exp\left(\frac{2\pi N\mathrm{i}}{N}\right)\right) = D_N, \tag{6.14}$$

equality (6.12) can be easily verified. In fact, by inserting $P_N = U_N D_N U_N^{-1}$ into $A_N = \sum_{n=-\nu}^{\nu} P_N^n \otimes Q_n$, one obtains

$$\begin{aligned} A_N &= \sum_{n=-\nu}^{\nu} \left(U_N D_N U_N^{-1}\right)^n \otimes (I_q Q_n I_q) \\ &= (U_N \otimes I_q)\left(\sum_{n=-\nu}^{\nu} D_N^n \otimes Q_n\right)\left(U_N^{-1} \otimes I_q\right), \end{aligned} \tag{6.15}$$

from which (6.12) follows immediately. □

Now we are ready to state the Compatibility Theorem, whose proof shall be given in the next section.

Theorem 6.1 (Compatibility Theorem, $X_r(q)$ version). Let $\{M_N\} \in X_r(q)$ be a repeat sequence and let $\{A_N\} \in X_{\#\alpha}(q)$ be the standard alpha sequence with $\{M_N\} - \{A_N\} \in X_\beta(q)$. Let F be the FS map associated with $\{A_N\}$. Then, we have

(i)

$$\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\left(F(\theta)\right) = \overline{\bigcup_{N \geqslant 1} \sigma(A_N)}. \tag{6.16}$$

(ii)

$$\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\left(F(\theta)\right) \subset \overline{\bigcup_{N \geqslant 1} \sigma(M_N)}. \tag{6.17}$$

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

Before proceeding to the next section, we give a proof of statement I in section 4.

Proof of statement I. The validity of statement I follows from part (iii) of theorem 6.1. □

7. Proof of the Compatibility Theorem

Before proving the Compatibility Theorem, we recall the following lemma, which was established and utilized in [27] for the first time to estimate quantum boundary effects in polymeric molecules. This lemma plays a crucial role in proving the Compatibility Theorem.

Lemma 7.1. Let $n \in \mathbb{Z}^+$ with $n \geqslant 2$, let $K = \{k_1, k_2, \dots, k_r\}$ be a subset of $\{1, 2, \dots, n\}$ consisting of r distinct elements $(1 \leqslant r < n)$, and let $L = \{1, 2, \dots, n\} \backslash K$. Let M and M' be $n \times n$ Hermitian matrices such that the ijth entries of M and M' coincide for all $(i, j) \in L \times L$, i.e., such that

$$\left(M - M'\right)_{ij} = 0 \tag{7.1}$$

for all $(i, j) \in L \times L$. Let $I = [a, b]$ be a closed interval which contains all the eigenvalues of both M and M'. Then, we have

$$\left|\operatorname{Tr} \varphi(M) - \operatorname{Tr} \varphi\left(M'\right)\right| \leqslant r V_I(\varphi) \tag{7.2}$$

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

Proof. This lemma is equivalent to lemma 2, proved in [27, chapter 7, p. 201]. (For the proofs essentially identical with the first proof in [27], the reader is referred to [28, p. 233] and [33, p. 62].) □

Remark 7.1. In [33], the above lemma 7.1 and the "α–β sequence decomposition approach" from the RST played a crucial role in investigating the asymptotics of eigenvalues of Toeplitz matrices and also to form, for the first time, a connection between the study of Toeplitz matrices and the RST (cf. [33] and references therein). The reader who is interested in the above mentioned connection is also referred to [34]. We note that section 5.8, entitled "Zizler, Zuidwijk, Taylor, Arimoto" in monograph [34], expounds the extension of the main results in [33] from eigenvalues to singular values for arbitrary band Toeplitz matrices.

Now we are ready to give a proof of the Compatibility Theorem (theorem 6.1) stated at the end of section 6.

Proof of theorem 6.1. (i) Let $\theta \in [0, 2\pi]$ and let $h_j(\theta)$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counting the multiplicity, arranged in the increasing order:

$$h_j(\theta) = \lambda_j\left(F(\theta)\right), \tag{7.3}$$

where $j \in \{1, \dots, q\}$. We know that

(a) The function $h_j : [0, 2\pi] \to \mathbb{R}$ defined by (7.3) is continuous for all $j \in \{1, \dots, q\}$.

(b) For $N \in \mathbb{Z}^+$, the eigenvalues of $qN \times qN$ real symmetric matrix A_N counting the multiplicity are:

$$h_1\left(\frac{2\pi 1}{N}\right), \dots, h_1\left(\frac{2\pi N}{N}\right), \dots, h_q\left(\frac{2\pi 1}{N}\right), \dots, h_q\left(\frac{2\pi N}{N}\right). \tag{7.4}$$

(Recall proposition 6.2.)

Let

$$L_N := \left\{ \frac{2\pi r}{N} \colon r \in \{1, \ldots, N\} \right\}, \tag{7.5}$$

$$L := \bigcup_{N \geqslant 1} L_N. \tag{7.6}$$

Thus, using the easily verifiable relations

$$h_j\left(\bigcup_{N \geqslant 1} L_N \right) = \bigcup_{N \geqslant 1} h_j(L_N), \tag{7.7}$$

$$\overline{L} = [0, 2\pi], \tag{7.8}$$

we get

$$\bigcup_{N \geqslant 1} \sigma(A_N) = \bigcup_{j=1}^{q} h_j(L), \tag{7.9}$$

$$\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big) = \bigcup_{j=1}^{q} h_j\big(\overline{L}\big). \tag{7.10}$$

Note that $h_j(\overline{L})$ is compact for all $j \in \{1, \ldots, q\}$, so we see that $\bigcup_{j=1}^{q} h_j(\overline{L})$ is a closed set in $\mathbb{R}$. Hence, $\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma(F(\theta))$ is a closed set in $\mathbb{R}$:

$$\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big) = \overline{\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big)}. \tag{7.11}$$

By (7.9)–(7.11), we obtain

$$\bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big) \supset \overline{\bigcup_{N \geqslant 1} \sigma(A_N)}. \tag{7.12}$$

The opposite inclusion follows easily from the fundamental properties of the closure operation and the relation $\overline{h_j(L)} \supset h_j(\overline{L})$, which is true by the continuity of h_j:

$$\begin{aligned} \overline{\bigcup_{N \geqslant 1} \sigma(A_N)} &= \overline{\bigcup_{j=1}^{q} h_j(L)} \\ &= \bigcup_{j=1}^{q} \overline{h_j(L)} \\ &\supset \bigcup_{j=1}^{q} h_j\big(\overline{L}\big) = \bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big). \end{aligned} \tag{7.13}$$

(ii) Let $k \in \{1, \dots, q\}$ and $\theta \in [0, 2\pi]$ be arbitrary. For the proof of (ii), we then have only to show that

$$h_k(\theta) \in \overline{\bigcup_{N \geqslant 1} \sigma(M_N)}. \tag{7.14}$$

Let I be a closed interval compatible with both $\{M_N\}$ and $\{A_N\}$. By (6.16), we see that the compatibility of I with $\{A_N\}$, i.e.,

$$\bigcup_{N \geqslant 1} \sigma(A_N) \subset I \tag{7.15}$$

implies that the following relations hold:

$$\bigcup_{j=1}^{q} h_j\big([0, 2\pi]\big) = \bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big) = \overline{\bigcup_{N \geqslant 1} \sigma(A_N)} \subset I. \tag{7.16}$$

So, the range of the function $h_j : [0, 2\pi] \to \mathbb{R}$ is contained in I for all $j \in \{1, \dots, q\}$. Hence, if U is any subset of $\mathbb{R}$, then for any $j \in \{1, \dots, q\}$, we have

$$h_j^{-1}(U \cap I) = h_j^{-1}(U) \cap h_j^{-1}(I) = h_j^{-1}(U) \cap [0, 2\pi] = h_j^{-1}(U). \tag{7.17}$$

Now we need the following

Proposition 7.1. The notation and assumptions being as above, if $\varphi \in BV(I)$, then

$$\operatorname{Tr} \varphi(M_N) - \operatorname{Tr} \varphi(A_N) = O(1) \tag{7.18}$$

as $N \to \infty$.

Proof of proposition 7.1. Since $\{M_N - A_N\} \in X_\beta(q)$, the conclusion directly follows from lemma 7.1. □

Let $\varepsilon > 0$ be arbitrary, let

$$U_\varepsilon := \big(h_k(\theta) - \varepsilon, h_k(\theta) + \varepsilon\big), \tag{7.19}$$

and define $\phi_\varepsilon \in BV(I)$ by

$$\phi_\varepsilon = \mathbf{1}_{U_\varepsilon \cap I}, \tag{7.20}$$

where $\mathbf{1}_{U_\varepsilon \cap I}$ stands for the characteristic function of the set $U_\varepsilon \cap I$.

We claim that

$$\operatorname{Tr} \phi_\varepsilon(A_N) \to \infty \tag{7.21}$$

as $N \to \infty$. Notice that (7.4) and (7.17) imply that

$$\operatorname{Tr} \phi_\varepsilon(A_N) = \sum_{j=1}^{q} \operatorname{Card}\big(L_N \cap h_j^{-1}(U_\varepsilon \cap I)\big)$$

$$= \sum_{j=1}^{q} \mathrm{Card}\big(L_N \cap h_j^{-1}(U_\varepsilon)\big)$$

$$\geqslant \mathrm{Card}\big(L_N \cap h_k^{-1}(U_\varepsilon)\big). \tag{7.22}$$

But, $h_k^{-1}(U_\varepsilon)$ is an open neighborhood of θ by the continuity of h_k, hence

$$\mathrm{Card}\big(L_N \cap h_k^{-1}(U_\varepsilon)\big) \to \infty \tag{7.23}$$

as $N \to \infty$. Thus, our claim is true.

By (7.18) and our claim just verified, we have

$$\mathrm{Tr}\, \phi_\varepsilon(M_N) \to \infty \tag{7.24}$$

as $N \to \infty$. This obviously shows that

$$U_\varepsilon \cap \sigma(M_N) \neq \varnothing, \tag{7.25}$$

for some $N \in \mathbb{Z}^+$, hence that

$$U_\varepsilon \cap \Big(\bigcup_{N \geqslant 1} \sigma(M_N)\Big) \neq \varnothing. \tag{7.26}$$

Since $\varepsilon > 0$ was arbitrary, (7.14) is true.

(iii) Suppose that I is a closed interval compatible with $\{M_N\}$. Then, we have

$$\bigcup_{N \geqslant 1} \sigma(M_N) \subset I. \tag{7.27}$$

Hence by using (i) and (ii), we see that

$$\bigcup_{N \geqslant 1} \sigma(A_N) \subset \overline{\bigcup_{N \geqslant 1} \sigma(A_N)} = \bigcup_{0 \leqslant \theta \leqslant 2\pi} \sigma\big(F(\theta)\big) \subset \overline{\bigcup_{N \geqslant 1} \sigma(M_N)} \subset \overline{I} = I. \tag{7.28}$$

This completes the proof of theorem 6.1. □

8. Concluding remarks

Among the proofs of the Functional ALT, with varying degrees of dependence on the Original ALT, is a proof that fully depends on the Original ALT, and at the same time, uses the well-known Banach–Steinhaus theorem. The proof along these lines requires the argument of the completeness of functional spaces; its details will be published elsewhere.

The present method of proving the Functional ALT for $X_r(q)$, via the Compatibility Theorem and theorem 4.3 can also be applied to the extended theoretical framework of the generalized repeat space $\mathscr{X}_r(q, d)$. We note that the Fukui conjecture, which was formulated in the setting of the original repeat space $X_r(q)$, continues to be of vital significance in view of the analogous statement in the extended setting of the generalized repeat space $\mathscr{X}_r(q, d)$. The development of the ALT in the latter setting shall be published elsewhere.

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