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Proof of the Fukui conjecture via resolution of singularities and related methods. I*

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The present article is the preliminary part of a series devoted to extending the foundation of the Asymptotic Linearity Theorems (ALTs), which prove the Fukui conjecture concerning the additivity problem of the zero-point vibrational energies of hydrocarbons. In this article, we establish a theorem, referred to as the $\mathscr{G}$ Boundedness Theorem, through which one can easily form a chain of logical implications that reduces a proof of the Fukui conjecture to that of the Piecewise Monotone Lemma (PML). This chain of logical implications serves as a basis throughout this series of articles. The PML, which has been indispensable for demonstrating any version of the ALTs and has required for its proof a mathematical language not generally known to chemists, is directly related to the theory of algebraic curves. Proofs of the original and enhanced versions of the PML are obtainable via resolution of singularities and related methods.

*Dedicated to the memory of Prof. Kenichi Fukui (1918–1998).

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1. Introduction

In recent works [1,2] concerning the Fukui conjecture, the following logical implications have been established between the validity of the conjecture and some fundamental theorems in the repeat space theory (RST) [3], called the Asymptotic Linearity Theorems (ALTs):

$$\text{Special Functional ALT} \Rightarrow \text{Functional ALT} \Rightarrow \text{the Fukui conjecture.} \quad (1.1)$$

We recall from [1] that the Fukui conjecture on the additivity problem of the zero-point vibrational energies of hydrocarbons played a prominent role in the initial development of the repeat space theory (RST) and that the conjecture continues to be of vital significance in the recent development of the theory of the generalized repeat space $\mathscr{X}_r(q,d)$ [4–7]. (For a review of the RST, the reader is referred to the paper [3] entitled "Note on the repeat space theory – its development and communications with Prof. Kenichi Fukui".)

The present article is the preliminary part of a series devoted to extending the foundation of the ALTs, which prove the Fukui conjecture, by using tools from algebraic geometry and related fields. The main purpose of this article is to establish what is called the $\mathscr{G}$ Boundedness Theorem, which is of major importance in this series of articles and is applicable to both the theory of the original repeat space $\mathscr{X}_r(q)$ (cf. [1,2] and references therein) and the theory of the generalized repeat space $\mathscr{X}_r(q,d)$. Through the $\mathscr{G}$ Boundedness Theorem, one can easily form a chain of logical implications that reduces a proof of the Fukui conjecture to that of the Piecewise Monotone Lemma (PML) (version 1) proved earlier (cf. lemma 2.1 in section 2). The PML, which has been indispensable for demonstrating any version of the ALTs and has required for its proof a mathematical language not generally known to chemists, is directly related to the theory of algebraic curves. In this article, we establish, for the first time, the following logical implications:

$$\begin{aligned}&\text{PML} \Rightarrow \mathscr{G}\text{ Boundedness Theorem} \Rightarrow \text{Special Functional ALT} \Rightarrow \\ &\text{Functional ALT} \Rightarrow \text{the Fukui conjecture.}\end{aligned} \quad (1.2)$$

This chain of logical implications serves as a basis throughout this series of articles.

In section 2, we establish the $\mathscr{G}$ Boundedness Theorem by using the PML, namely, we obtain the following implication:

$$\text{PML} \Rightarrow \mathscr{G}\text{ Boundedness Theorem.} \quad (1.3)$$

In section 3, we demonstrate the following implication:

$$\mathscr{G}\text{ Boundedness Theorem} \Rightarrow \text{Special Functional ALT.} \tag{1.4}$$

Consequently, we get (1.2) by combining (1.1), (1.3), and (1.4).

In subsequent parts of this series, a new version of PML, which is more powerful than the PML version 1, will be developed by using resolution of singularities and related methods.

2. The $\mathscr{G}$ Boundedness Theorem

Throughout, let $\mathbb{Z}^+, \mathbb{R}$, and $\mathbb{C}$ denote, respectively, the set of all positive integers, real numbers, and complex numbers.

To formulate the $\mathscr{G}$ Boundedness Theorem described in section 1, we need the following definition and notation.

Definition 2.1. Let S_1 and S_2 be nonempty subsets of $\mathbb{R}$. A function f: $S_1 \to S_2$ is said to be *nondecreasing* if $x_1 \leqslant x_2$ implies $f(x_1) \leqslant f(x_2)$ for all $x_1, x_2 \in S_1$. A function f: $S_1 \to S_2$ is said to be *nonincreasing* if $x_1 \leqslant x_2$ implies $f(x_2) \leqslant f(x_1)$ for all $x_1, x_2 \in S_1$. A function f: $S_1 \to S_2$ is said to be *monotone* if it is either nondecreasing or nonincreasing.

Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. A function $f: I \to \mathbb{R}$ is said to be *piecewise monotone* if there exists a finite partition

$$a = x_0 < x_1 < \cdots < x_n = b \quad (n \in \mathbb{Z}^+) \tag{2.1}$$

of the interval I such that the restriction $f|[x_{i-1}, x_i]$ is monotone for all $i \in \{1, \ldots, n\}$. In this case, f is said to have n-partition of monotonicity.

A real-valued function on a subset $S \subset \mathbb{R}$ is called *real analytic on* S if it is the restriction to S of a function which is real analytic on some open set $O \supset S$.

Notation 2.1. Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$.
If f: $I \to \mathbb{R}$ is piecewise monotone, let

$$\mathrm{Mo}(f) := \min\{n \in \mathbb{Z}^+ : f \text{ has } n\text{-partition of monotonicity}\}. \tag{2.2}$$

The $\mathrm{Mo}(f)$ is called the *monotonicity number of* f.
If $f: I \to \mathbb{R}$ is not piecewise monotone, let

$$\mathrm{Mo}(f) = \infty. \tag{2.3}$$

$C^\omega(I)$: the ring (UFD) of all real analytic functions defined on I.
$C^\omega(I)[\lambda]$: the polynomial ring (UFD) over $C^\omega(I)$ in the indeterminate λ.
$C(I)$: the ring of all real-valued continuous functions defined on I.
$C(I)[\lambda]$: the polynomial ring over $C(I)$ in the indeterminate λ.

$\mathbb{R}[\lambda]$: the polynomial ring (UFD) over $\mathbb{R}$ in the indeterminate λ.
For each $\theta \in I$, let $\mathrm{Ev}_\theta : C(I)[\lambda] \to \mathbb{R}[\lambda]$ be the ring homomorphism defined by

$$\mathrm{Ev}_\theta(c_0\lambda^n + c_1\lambda^{n-1} + \cdots + c_n) = c_0(\theta)\lambda^n + c_1(\theta)\lambda^{n-1} + \cdots + c_n(\theta). \quad (2.4)$$

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

$$V_I(\varphi) = \sup_\Delta \sum_{i=1}^{n} |\varphi(t_i) - \varphi(t_{i-1})|. \quad (\Delta : a = t_0 \leqslant t_1 \leqslant \cdots \leqslant t_n = b) \quad (2.5)$$

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

$$\|\varphi\| = \sup\{|\varphi(t)| : t \in I\} + V_I(\varphi). \quad (2.6)$$

Remark 2.1. It is not difficult to verify that $C^\omega(I)$ is a UFD (unique factorization domain) and hence that $C^\omega(I)[\lambda]$ is a UFD. It is easy to see that $C^\omega(I) \subset C(I)$, $C^\omega(I)[\lambda] \subset C(I)[\lambda]$, and that neither $C(I)$ nor $C(I)[\lambda]$ is a UFD. For the fundamental properties of UFDs, the reader is referred to, e.g. [8,9].

Now we are ready to state and prove the $\mathscr{G}$ Boundedness Theorem.

Theorem 2.1. ($\mathscr{G}$ Boundedness Theorem). Let $\tilde{a}$, $\tilde{b} \in \mathbb{R}$ with $\tilde{a} < \tilde{b}$ and let $\tilde{I} = [\tilde{a}, \tilde{b}]$. Let $p \in C^\omega(\tilde{I})[\lambda]$ be a monic polynomial of degree $q \in \mathbb{Z}^+$ given by

$$p = \lambda^q + c_1\lambda^{q-1} + \cdots + c_q. \quad (2.7)$$

Suppose that for any $\theta \in \tilde{I}$, the polynomial

$$\mathrm{Ev}_\theta(p) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta) \quad (2.8)$$

over the field $\mathbb{R}$ has q real roots. Define the mapping f: $\tilde{I} \to \mathbb{R}[\lambda]$ by

$$f(\theta) = \mathrm{Ev}_\theta(p), \quad (2.9)$$

and let $r_j(f(\theta))$ denote the jth root of $f(\theta)$ counted with multiplicity, arranged in the increasing order, where $j \in \{1, \cdots, q\}$. Let a, $b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. Suppose that I contains all the roots of $f(\theta)$ for all $\theta \in \tilde{I}$. Then, the following statements are true:

(i) For each $\varphi \in CBV(I)$, the function $\theta \mapsto \sum_{j=1}^{q} \varphi(r_j(f\theta)))$ defined on $\tilde{I}$ is real-valued continuous and of bounded variation, i.e., an element of $CBV(\tilde{I})$.

(ii) Define the linear operator $\mathscr{G}: CBV(I) \to CBV(\tilde{I})$ by

$$\mathscr{G}(\varphi)(\theta) = \sum_{j=1}^{q} \varphi(r_j(f(\theta))). \tag{2.10}$$

Then, $\mathscr{G}$ is bounded:

$$\|\mathscr{G}\| < \infty. \tag{2.11}$$

Proof. (i) Since $CBV(\tilde{I})$ is a linear space, it suffices to prove that for each $j \in \{1, \ldots, q\}$ and $\varphi \in CBV(I)$, the function $\theta \mapsto \varphi(r_j(f(\theta)))$ defined on $\tilde{I}$ is real-valued continuous and of bounded variation.

Fix any $j \in \{1, \ldots, q\}$ and define the function λ_j: $\tilde{I} \to \mathbb{R}$ by

$$\lambda_j(\theta) = r_j(f(\theta)). \tag{2.12}$$

(To see that the function λ_j is well-defined, recall the assumption that polynomial (2.8) has always q real roots.)

First, under the assumption of the theorem, note that the coefficients of $p = \lambda^q + c_1\lambda^{q-1} + \cdots + c_q \in C^\omega(\tilde{I})[\lambda]$ are real-analytic, hence real-valued continuous functions defined on $\tilde{I}$. This fact and proposition 2.1 following theorem 2.1 easily imply that the λ_j is continuous:

$$\lambda_j \in C(\tilde{I}). \tag{2.13}$$

Consequently, the function $\theta \mapsto \varphi(\lambda_j(\theta))$ defined on $\tilde{I}$ is real-valued continuous whenever $\varphi \in CBV(I)$. (To see that this function is well-defined, recall the assumption that I contains all the roots of $f(\theta)$ for all $\theta \in \tilde{I}$.)

Second, note that the lemma 2.1 (PML) given at the end of this section implies that the λ_j is piecewise monotone:

$$\mathrm{Mo}(\lambda_j) < \infty. \tag{2.14}$$

Consider any partition of the interval $\tilde{I} = [\tilde{a}, \tilde{b}]$

$$\Delta: \tilde{a} = \theta_0 \leqslant \theta_1 \leqslant \cdots \leqslant \theta_n = \tilde{b}. \tag{2.15}$$

Let φ be any element of $CBV(I)$. We then obtain the following inequality:

$$\sum_{k=1}^{n} |\varphi(\lambda_j(\theta_k)) - \varphi(\lambda_j(\theta_{k-1}))| \leqslant \mathrm{Mo}(\lambda_j) V_I(\varphi). \tag{2.16}$$

Consequently, the function $\theta \mapsto \varphi(\lambda_j(\theta))$ defined on $\tilde{I}$ is of bounded variation whenever $\varphi \in CBV(I)$.

(ii) Let $\theta_0, \theta_1, \ldots, \theta_n$ be as in (2.15). Observe that

$$\sum_{k=1}^{n} |\mathscr{G}(\varphi)(\theta_k) - \mathscr{G}(\varphi)(\theta_{k-1})| \leqslant \sum_{j=1}^{q}\sum_{k=1}^{n} |\varphi(\lambda_j(\theta_k)) - \varphi(\lambda_j(\theta_{k-1}))|$$
$$\leqslant \left(\sum_{j=1}^{q} \mathrm{Mo}(\lambda_j)\right) V_I(\varphi). \tag{2.17}$$

Straight from the definition of the total variation, we get

$$V_{\tilde{I}}(\mathscr{G}(\varphi)) \leqslant \left(\sum_{j=1}^{q} \mathrm{Mo}(\lambda_j)\right) V_I(\varphi). \tag{2.18}$$

By (2.18) and the easily verifiable relation:

$$\sup\{|\mathscr{G}(\varphi)(\theta)| : \theta \in \tilde{I}\} \leqslant q \sup\{|\varphi(t)| : t \in I\}, \tag{2.19}$$

one obtains immediately

$$\|\mathscr{G}(\varphi)\| \leqslant \max\left\{q, \sum_{j=1}^{q} \mathrm{Mo}(\lambda_j)\right\} \|\varphi\| \leqslant \left(\sum_{j=1}^{q} \mathrm{Mo}(\lambda_j)\right) \|\varphi\| \tag{2.20}$$

for all $\varphi \in CBV(I)$. This shows that $\mathscr{G}$ is bounded:

$$\|\mathscr{G}\| \leqslant \sum_{j=1}^{q} \mathrm{Mo}(\lambda_j) < \infty. \tag{2.21}$$

□

Proposition 2.1. Let $a,b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. Let $p \in C(I)[\lambda]$ be a monic polynomial of degree $q \in \mathbb{Z}^+$ given by

$$p = \lambda^q + c_1\lambda^{q-1} + \cdots + c_q. \tag{2.22}$$

Suppose that for any $\theta \in I$, the polynomial

$$\mathrm{Ev}_\theta(p) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta) \tag{2.23}$$

over the field $\mathbb{R}$ has q real roots, which we denote by $\lambda_1(\theta) \leqslant \lambda_2(\theta) \leqslant \cdots \leqslant \lambda_q(\theta)$. Then, all the λ_j's are continuous, i.e.,

$$\lambda_j \in C(I) \tag{2.24}$$

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

Proof. Fix any $\theta \in I$, and fix any sequence $\theta_n \in I$ that converges to θ. For the proof of the proposition, we have only to verify that for each $j \in \{1, \dots, q\}$,

$$\lambda_j(\theta_n) \to \lambda_j(\theta) \tag{2.25}$$

as $n \to \infty$.

Let $g, g_n : \mathbb{C} \to \mathbb{C}$ be the polynomial functions defined by

$$g(\lambda) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta), \tag{2.26}$$

$$g_n(\lambda) = \lambda^q + c_1(\theta_n)\lambda^{q-1} + \cdots + c_q(\theta_n) \quad (n \in \mathbb{Z}^+). \tag{2.27}$$

Let K be any compact subset of $\mathbb{C}$.

First, note that for each $j \in \{1, \dots, q\}$, we have

$$\sup_{\lambda \in K} |\lambda^{q-j}| < \infty \tag{2.28}$$

since the function $\lambda \mapsto \lambda^{q-j}$ is continuous on compact set K. Second, note that for each $j \in \{1, \dots, q\}$, we have

$$|c_j(\theta) - c_j(\theta_n)| \to 0 \tag{2.29}$$

as $n \to \infty$, since c_j is continuous at θ.

We now see that

$$0 \leqslant \sup_{\lambda \in K} |g(\lambda) - g_n(\lambda)| \leqslant \sum_{j=1}^{q} |c_j(\theta) - c_j(\theta_n)| \sup_{\lambda \in K} |\lambda^{q-j}| \to 0, \tag{2.30}$$

hence that

$$\sup_{\lambda \in K} |g(\lambda) - g_n(\lambda)| \to 0 \tag{2.31}$$

as $n \to \infty$. Thus, g_n converges to g uniformly on compact subsets of $\mathbb{C}$.

Let k denote the number of elements in the set $\{\lambda_1(\theta), \dots, \lambda_q(\theta)\}$, i.e.,

$$k = \text{Card } \{\lambda_1(\theta), \dots, \lambda_q(\theta)\}, \tag{2.32}$$

let $\mu_1 < \cdots < \mu_k$ be such that

$$\{\mu_1, \dots, \mu_k\} = \{\lambda_1(\theta), \dots, \lambda_q(\theta)\}. \tag{2.33}$$

For each $j \in \{1, \dots, k\}$, let m_j denote the multiplicity of root μ_j:

$$m_j = \text{Card } \{i \in \{1, \dots, q\} : \mu_j = \lambda_i(\theta)\}. \tag{2.34}$$

Let d be the minimum length of intervals $[\mu_j, \mu_{j+1}]$:

$$d = \min\{\mu_{j+1} - \mu_j : j \in \{1, \dots, k-1\}\}. \tag{2.35}$$

Given $\varepsilon > 0$ with $d/3 > \varepsilon$, then for any $i \in \{1, \dots, k\}$ and for any λ on the sphere $\{\lambda \in \mathbb{C}: |\lambda - \mu_i| = \varepsilon\}$, we have

$$g(\lambda) \neq 0. \tag{2.36}$$

Now we may apply the following Hurwitz's Theorem, and deduce that for any $i \in \{1, \dots, k\}$, there exists an integer $n_0(i)$ such that for all $n \geqslant n_0(i)$, the polynomial g_n has m_i zeros (counted with multiplicity) in the open disc $D(\mu_i, \varepsilon) = \{\lambda \in \mathbb{C}: |\lambda - \mu_i| < \varepsilon\}$. Let

$$N := \max\{n_0(i) : i \in \{1, \dots, k\}\}. \tag{2.37}$$

Then, we see that for any $i \in \{1, \dots, k\}$ and any $n \geqslant N, g_n$ has m_i zeros (counted with multiplicity) in the open disc $D(\mu_i, \varepsilon)$. This implies that for any $j \in \{1, \dots, q\}$

$$\lambda_j(\theta_n) \in \{\lambda \in \mathbb{R}: |\lambda - \lambda_j(\theta)| < \varepsilon\} \tag{2.38}$$

for all $n \geqslant N$, showing that $\lambda_j \in C(I)$. □

Hurwitz's Theorem. Let $G \subset \mathbb{C}$ be a region, let $H(G)$ denote the set of all complex-valued analytic functions on G, and let $f, f_n \in H(G)$ be such that f_n converges to f uniformly on compact subsets of G. Let $\overline{D}(a, r) = \{z \in \mathbb{C}: |z - a| \leqslant r\}$ be a closed disc contained in G. Suppose that $f \not\equiv 0$ and $f(z) \neq 0$ for $|z - a| = r$. Then, there is an integer n_0 such that for all $n \geqslant n_0$, f and f_n have the same number of zeros in the open disc $D(a, r) = \{z \in \mathbb{C}: |z - a| < r\}$ (counted with multiplicity).

(Cf. for example, [10].)

Remark 2.2. More general forms of proposition 2.1 are well known. We have formulated proposition 2.1 for our immediate purpose restricting to the case where the coefficients of polynomial p are all in $C(I)$. We remark that the conclusion of Hurwitz's Theorem easily follows from Rouché's Theorem and that proposition 2.1 can also be proved by using the latter theorem.

Lemma 2.1. (Piecewise Monotone Lemma (PML) version 1). Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. Let $p \in C^{\omega}(I)[\lambda]$ be a monic polynomial of degree $q \in \mathbb{Z}^+$ given by

$$p = \lambda^q + c_1 \lambda^{q-1} + \cdots + c_q. \tag{2.39}$$

Suppose that for any $\theta \in I$, the polynomial

$$\mathrm{Ev}_\theta(p) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta) \tag{2.40}$$

over the field $\mathbb{R}$ has q real roots, which we denote by $\lambda_1(\theta) \leqslant \lambda_2(\theta) \leqslant \cdots \leqslant \lambda_q(\theta)$. Then, all the λ_j's are piecewise monotone, i.e.,

$$\mathrm{Mo}(\lambda_j) < \infty \tag{2.41}$$

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

Proof. This is equivalent to lemma 4 in [11]. □

3. Reduction of a proof of the Special Functional Asymptotic Linearity Theorem to that of the $\mathscr{G}$ Boundedness Theorem

For the above stated goal of the reduction, we begin this section by preparing the following propositions 3.1 and 3.2. The reader is referred to [1,2] for the definitions of notions and symbols in these propositions and the subsequent theorems.

Proposition 3.1. Suppose that $\{A_N\} \in X_{\#\alpha}(q)$ and that A_N is given by

$$A_N = \sum_{n=-v}^{v} P_N^n \otimes Q_n, \tag{3.1}$$

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

$$F(\theta) = \sum_{n=-v}^{v} (\exp(in\theta)) Q_n, \tag{3.2}$$

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

$$h_j(\theta) = \lambda_j(F(\theta)), \tag{3.3}$$

where $\lambda_j(F(\theta))$ denotes the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with 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:

$$\begin{aligned}(U_N \otimes I_q)^{-1} A_N (U_N \otimes I_q) \\ = \text{B-diag}(F(2\pi/N), F(2\pi 2/N), \ldots, F(2\pi N/N)),\end{aligned} \tag{3.4}$$

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

$$(U_N)_{mn} = N^{-1/2} \exp(2\pi mni/N), \tag{3.5}$$

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

(iii) If I is a closed interval compatible with $\{A_N\}$, and if φ is a real-valued function defined on I, then

$$\mathrm{Tr}\varphi(A_N) = \sum_{r=1}^{N}\sum_{j=1}^{q}\varphi(\lambda_j(F(2\pi r/N))). \tag{3.6}$$

Proof. Both (i) and (ii) were proved in [12]. (The proof of (ii) was reproduced in [1].) We thus prove here only part (iii):

Since A_N and the right-hand side of equality (3.4) are similar, the eigenvalues of A_N and those of the block-diagonal matrix coincide; thus we have

$$\mathrm{Tr}\varphi(A_N) = \sum_{i=1}^{qN}\varphi(\lambda_i(A_N)) = \sum_{r=1}^{N}\sum_{j=1}^{q}\varphi(\lambda_j(F(2\pi r/N))), \tag{3.7}$$

where $\lambda_i(A_N)$ denotes the ith eigenvalue of A_N counted with multiplicity, arranged in the increasing order. □

Proposition 3.2. Let $\tilde{I} = [0, 2\pi]$, define the sequence of linear functionals $\tilde{\beta}_N{:}CBV(\tilde{I}) \to \mathbb{R}$ by

$$\tilde{\beta}_N(\varphi) = \left(\sum_{r=1}^{N}\varphi(2\pi r/N)\right) - (N/(2\pi))\int_0^{2\pi}\varphi(\theta)d\theta. \tag{3.8}$$

Then, we have

$$\sup\{\|\tilde{\beta}_N\| : N \geqslant 1\} \leqslant 1. \tag{3.9}$$

Proof. Observe that

$$\begin{aligned} |\tilde{\beta}_N(\varphi)| &= \left|\sum_{r=1}^{N}\varphi(2\pi r/N) - (N/(2\pi))\int_0^{2\pi}\varphi(\theta)d\theta\right| \qquad (3.10)\\ &\leqslant (N/(2\pi))\sum_{r=1}^{N}\int_{2\pi(r-1)/N}^{2\pi r/N}|\varphi(2\pi r/N) - \varphi(\theta)|d\theta \\ &\leqslant (N/(2\pi))\sum_{r=1}^{N}\int_{2\pi(r-1)/N}^{2\pi r/N}V_{[2\pi(r-1)/N, 2\pi r/N]}(\varphi)d\theta \\ &\leqslant V_{\tilde{I}}(\varphi) \\ &\leqslant \sup\{|\varphi(t)| : t \in \tilde{I}\} + V_{\tilde{I}}(\varphi) = \|\varphi\|, \end{aligned}$$

for all $\varphi \in CBV(\tilde{I})$ and $N \in \mathbb{Z}^+$, from which the conclusion follows immediately. □

Theorem 3.1. (Special Functional ALT, $X_\alpha(q)$ version). Let $\{A_N\} \in X_{\#\alpha}(q)$ be a fixed standard α sequence, let I be a fixed closed interval compatible with $\{A_N\}$. Then, there exist functionals $\alpha, \beta \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ such that

$$\mathrm{Tr}\varphi(A_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{3.11}$$

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

Before proving theorem 3.1, we note that the following theorem $3.1^{\#}$, which is a weaker version of theorem 3.1, is easily proved.

Theorem 3.1.$^{\#}$ Let $\{A_N\} \in X_{\#\alpha}(q)$ be a fixed standard α sequence, let I be a fixed closed interval compatible with $\{A_N\}$. Then, there exists a functional $\alpha \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ such that

$$\mathrm{Tr}\varphi(A_N) = \alpha(\varphi)N + o(N) \tag{3.12}$$

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

Proof. The conclusion easily follows from the fact that $X_{\#\alpha}(q) \subset X_{\mathrm{r}}(q)$ and the former part of the proof of the Functional ALT in [1], the part which involves propositions (a1), (a2), (a3), and (a4). □

Proof of theorem 3.1. Let $\alpha \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ be as in theorem $3.1^{\#}$ and note that α whose existence is asserted in theorem $3.1^{\#}$ is unique since

$$\alpha(\varphi) = \lim_{N\to\infty} [\mathrm{Tr}\varphi(A_N)]/N \tag{3.13}$$

for all $\varphi \in AC(I)$. Define the sequence of linear functionals $\beta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ by

$$\beta_N(\varphi) = \mathrm{Tr}\varphi(A_N) - \alpha(\varphi)N. \tag{3.14}$$

Suppose that for each $N \in \mathbb{Z}^+$, we are given an element

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

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

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

(cf. [13]), consider the following four propositions:

(t1) for all $\varphi \in P(I)$, exists in $\mathbb{R}$,

(t2) $\sup\{\|\tau_N\|: N \leqslant 1\} < \infty$, (t3) for all $\varphi \in AC(I), \lim_{N\to\infty} \tau_N(\varphi)$ exists in $\mathbb{R}$,

(t4) $\tau : AC(I) \to \mathbb{R}$ defined by

$$\tau(\varphi) = \lim_{N\to\infty} \tau_n(\varphi) \tag{3.17}$$

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

By (3.16) and theorem 4.3(iii) in [1], we see that (t1) and (t2) imply (t3) and (t4).

Set $\tau_N = \beta_N$ and notice that for the proof of the theorem, it remains to prove that

$$\beta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R}) \tag{3.18}$$

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

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

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

But, (b1) is an immediate consequence of theorem 4.1 in [1]. Therefore, the proof of the theorem is reduced to the following theorem 3.2. □

Theorem 3.2. (β_N Uniform Boundedness Theorem, $X_{\#\alpha}(q)$ version). Let $\{A_N\} \in X_{\#\alpha}(q)$ be a fixed standard α sequence, let I be a fixed closed interval compatible with $\{A_N\}$. Define the sequences of linear functionals $\beta_N : AC(I) \to \mathbb{R}$ by

$$\beta_N(\varphi) = \mathrm{Tr}\varphi(A_N) - \alpha(\varphi)N, \tag{3.19}$$

where $\alpha(\varphi) := \lim_{N\to\infty}[\mathrm{Tr}\varphi(A_N)]/N$.

Then,

$$\beta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R}) \tag{3.20}$$

for all $N \in \mathbb{Z}^+$, and we have

$$\sup\{\|\beta_N\| : N \geqslant 1\} < \infty. \tag{3.21}$$

Proof. To see that $\beta_N \in AC(I)^*$, note that the following relations

$$\begin{aligned}
&|\beta_N(\varphi)| \\
&\leqslant |\mathrm{Tr}\varphi(M_N)| + |\alpha(\varphi)N| \\
&\leqslant 2qN(\sup\{|\varphi(t)| : t \in I\}) \\
&\leqslant 2qN(\sup\{|\varphi(t)| : t \in I\} + V_I(\varphi)) = 2qN\|\varphi\|
\end{aligned} \tag{3.22}$$

hold for all $\varphi \in AC(I)$ and $N \in \mathbb{Z}^+$.

Let F be the FS map associated with $\{A_N\}$. Recall theorem 6.1 (Compatibility Theorem) in [1], and notice that since I is compatible with $\{A_N\}$ by the assumption, I is also compatible with F, i.e., I contains all the eigenvalues of $F(\theta)$ for all $\theta \in \mathbb{R}$. Let $\tilde{I} = [0, 2\pi]$ and define the linear operator $G : CBV(I) \to CBV(\tilde{I})$ by

$$G(\varphi)(\theta) = \sum_{j=1}^{q} \varphi(\lambda_j(F(\theta))), \tag{3.23}$$

where $\lambda_j(F(\theta))$ denotes the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with multiplicity, arranged in the increasing order. (Note: To see that G is well-defined, see theorem 3.3(i) given below.)

Let G_0 be the restriction of G to the linear subspace $AC(I)$:

$$G_0 := G|AC(I). \tag{3.24}$$

Then, proposition 3.1(iii) implies that

$$\mathrm{Tr}\varphi(A_N) = \sum_{r=1}^{N} G_0(\varphi)(2\pi r/N) \tag{3.25}$$

for all $\varphi \in AC(I)$, hence that

$$\alpha(\varphi) = \lim_{N\to\infty} [\mathrm{Tr}\varphi(A_N)]/N = (1/(2\pi)) \int_0^{2\pi} G_0(\varphi)(\theta)d\theta \tag{3.26}$$

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

Define $\tilde{\beta}_N : CBV(\tilde{I}) \to \mathbb{R}$ as in proposition 3.2, and notice that

$$\beta_N = \tilde{\beta}_N \circ G_0 \tag{3.27}$$

for all $N \in \mathbb{Z}^+$. This and proposition 3.2 imply that

$$\|\beta_N\| \leqslant \|\tilde{\beta}_N\| \|G_0\| \leqslant \|G_0\| \leqslant \|G\| \tag{3.28}$$

for all $N \in \mathbb{Z}^+$. By the following theorem, theorem 3.3, inequality (3.21) holds. □

Theorem 3.3. (G Boundedness Theorem). Let $q \in \mathbb{Z}^+$, let v be a nonnegative integer, and let $Q_{-v}, Q_{-v+1}, \ldots, Q_v$ be $q \times q$ real matrices such that Q_{-n} is the transpose of Q_n for all $n \in \{0, 1, \ldots, v\}$. For each $\theta \in \mathbb{R}$, let $F(\theta)$ denote the $q \times q$ Hermitian matrix defined by

$$F(\theta) = \sum_{n=-v}^{v} (\exp(in\theta))Q_n. \tag{3.29}$$

For each $j \in \{1, \ldots, q\}$ and $\theta \in \mathbb{R}$, let $\lambda_j(F(\theta))$ denote the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with multiplicity, arranged in the increasing order. Let $a, b \in \mathbb{R}$ with $a < b$ and let $I = [a, b]$. Let $\tilde{a}, \tilde{b} \in \mathbb{R}$ with $\tilde{a} < \tilde{b}$ and let $\tilde{I} = [\tilde{a}, \tilde{b}]$. Suppose that I contains all the eigenvalues of $F(\theta)$ for all $\theta \in \tilde{I}$. Then, the following statements are true:

(i) For each $\varphi \in CBV(I)$, the function $\theta \mapsto \sum_{j=1}^{q} \varphi(\lambda_j(F(\theta)))$ defined on $\tilde{I}$ is real-valued continuous and of bounded variation, i.e., an element of $CBV(\tilde{I})$.

(ii) Define the linear operator $G : CBV(I) \to CBV(\tilde{I})$ by

$$G(\varphi)(\theta) = \sum_{j=1}^{q} \varphi(\lambda_j(F(\theta))). \tag{3.30}$$

Then, G is bounded:

$$\|G\| < \infty. \tag{3.31}$$

Proof. Consider the characteristic equation

$$\det(\lambda I_q - F(\theta)) = 0, \tag{3.32}$$

where I_q denotes the $q \times q$ unit matrix. For each $\theta \in \mathbb{C}$, the left-hand side can be written as a monic polynomial of degree q:

$$\det(\lambda I_q - F(\theta)) = \lambda^q + d_1(\theta)\lambda^{q-1} + \cdots + d_q(\theta). \tag{3.33}$$

In view of the analyticity of each entry of $F(\theta)$ and the definition of the determinant, $d_j : \theta \mapsto d_j(\theta)$ are obviously all analytic functions on $\mathbb{C}$. They are real-valued on $\mathbb{R}$ since for each $\theta \in \mathbb{R}$, all the roots of equation (3.32) are real. In fact, for each $\theta \in \mathbb{R}$, the left-side of equation (3.32) can be expressed by

$$\det(\lambda I_q - F(\theta)) = \prod_{j=1}^{q} (\lambda - \lambda_j(F(\theta))), \tag{3.34}$$

where $\lambda_j(F(\theta))$, the jth eigenvalue of the Hermitian matrix $F(\theta)$ counted with multiplicity, arranged in the increasing order, is clearly real. [Note: If $U(\theta)$ is a unitary matrix such that $U(\theta)^{-1} F(\theta) U(\theta) = D(\theta)$ where $D(\theta) = \mathrm{diag}(\lambda_1(F(\theta)), \ldots, \lambda_q(F(\theta)))$, then $\det(\lambda I_q - F(\theta)) = \det(U(\theta)) \det(\lambda I_q - D(\theta)) \det(U(\theta)^{-1}) = \det(\lambda I_q - D(\theta)) = \prod_{j=1}^{q} (\lambda - \lambda_j(F(\theta)))$.]

For each $j \in \{1, \ldots, q\}$, let c_j denote the restriction of d_j to the interval $\tilde{I}$:

$$c_j := d_j | \tilde{I}, \tag{3.35}$$

and let $p \in C^{\omega}(\tilde{I})[\lambda]$ be the monic polynomial of degree q given by

$$p = \lambda^q + c_1\lambda^{q-1} + \cdots + c_q. \tag{3.36}$$

Then, for any $\theta \in \tilde{I}$, the polynomial

$$\mathrm{Ev}_\theta(p) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta) \tag{3.37}$$

over the field $\mathbb{R}$ has q real roots: $\lambda_1(F(\theta)) \leqslant \cdots \leqslant \lambda_q(F(\theta))$. Define the mapping $f : \tilde{I} \to \mathbb{R}[\lambda]$ by

$$f(\theta) = \mathrm{Ev}_\theta(p), \tag{3.38}$$

and let $r_j(f(\theta))$ denote the jth root of $f(\theta)$ counted with multiplicity, arranged in the increasing order, where $j \in \{1, \ldots, q\}$. Then, we obviously have

$$r_j(f(\theta)) = \lambda_j(F((\theta))) \tag{3.39}$$

for all $j \in \{1, \ldots, q\}$ and $\theta \in \tilde{I}$. Now the conclusion easily follows from theorem 2.1, the $\mathcal{G}$ Boundedness Theorem. □

4. Concluding remarks

The notation and assumptions being as in theorem 3.3 (G Boundedness Theorem), for each $j \in \{1, \ldots, q\}$ define the function $\hat{\lambda}_j : \tilde{I} \to \mathbb{R}$ by

$$\hat{\lambda}_j(\theta) = \lambda_j(F(\theta)). \tag{4.1}$$

Recall the last inequalities

$$\|\mathcal{G}\| \leqslant \sum_{j=1}^{q} \mathrm{Mo}(\lambda_j) < \infty \tag{4.2}$$

in the proof of theorem 2.1 ($\mathcal{G}$ Boundedness Theorem), which uses lemma 2.1 (PML), and notice that the following inequalities hold in the setting of theorem 3.3.

$$\|G\| \leqslant \sum_{j=1}^{q} \mathrm{Mo}(\hat{\lambda}_j) < \infty. \tag{4.3}$$

Now in the setting of theorem 3.2 (β_N Uniform Boundedness Theorem) and its proof, for each $j \in \{1, \ldots, q\}$ define the function $\hat{\lambda}_j : \tilde{I} \to \mathbb{R}$ by (4.1), and recall inequalities (3.28) so that by inequalities (4.3) we see that

$$\|\beta_N\| \leqslant \|G\| \leqslant \sum_{j=1}^{q} \mathrm{Mo}(\hat{\lambda}_j) < \infty \tag{4.4}$$

for all $N \in \mathbb{Z}^{+}$. Note that the proof of theorem 3.1 (Special Functional ALT) was reduced to proving the fact that (b2) $\sup\{\|\beta_N\|{:}N \cdot 1 \ <\}\infty$. Thus, by the above argument and inequalities (4.4), one can easily overview the following logical implications.

PML $\Rightarrow \mathscr{G}$ Boundedness Theorem $\Rightarrow G$ Boundedness Theorem $\Rightarrow$
Special Functional ALT. (4.5)

In section 3, we have reduced a proof of the Special Functional Asymptotic Linearity Theorem to that of the $\mathscr{G}$ Boundedness Theorem, via the G Boundedness Theorem. As can be seen in the definitions of $\lambda_j(F(\theta))$ and $r_j(f(\theta))$ and in the proof of the G Boundedness Theorem, the $\mathscr{G}$ Boundedness Theorem is a generalization of the G Boundedness Theorem from the jth eigenvalue of the $q \times q$ Hermitian matrix:

$$F(\theta) = \sum_{n=-v}^{v} (\exp(in\theta))Q_n, \tag{4.6}$$

to the jth root of the polynomial of degree q with q real roots:

$$f(\theta) = \lambda^q + c_1(\theta)\lambda^{q-1} + \cdots + c_q(\theta), \tag{4.7}$$

where $c_1, \ldots, c_q$ are all real analytic functions on $\tilde{I} = [\tilde{a}, \tilde{b}]$.

The following theorem from [4] and its generalized analogues play an important role in the development of the theory of generalized repeat space $\mathscr{X}_r(q, d)$ [4–7].

Theorem I. Let $\tilde{a}$, $\tilde{b}$, a, $b \in \mathbb{R}$ with $\tilde{a} < \tilde{b}$ and $a < b$. Let $\tilde{I} = [\tilde{a}, \tilde{b}]$, let $I = [a, b]$, and let $x(N, r) = \tilde{a} + (\tilde{b} - \tilde{a})r/N$. Let q be a fixed positive integer and let $u_1, u_2, \ldots, u_q$ be fixed real analytic functions defined on $\tilde{I}$. Suppose that I contains all the images of $\tilde{I}$ under the functions $u_1, u_2, \ldots, u_q$. Let $E_N{:}AC(I) \to \mathbb{R}$ be the sequence of linear functionals defned by

$$E_N(\varphi) = \sum_{r=1}^{N} \sum_{j=1}^{q} \varphi(u_j(x(N, r))). \tag{4.8}$$

Then, there exist functionals $\alpha, \beta \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ such that

$$E_N(\varphi) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{4.9}$$

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

As the final remark, we note that the $\mathscr{G}$ Boundedness Theorem, which is of fundamental importance for the reduction of a proof of the Functional ALT, will be also utilized for establishing one of the generalized analogues of the above theorem I. The details along these lines will be published elsewhere.

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References

[1] S. Arimoto, J. Math. Chem. 34 (2003) 259–285.
[2] S. Arimoto, J. Math. Chem. 34 (2003) 287–296.
[3] S. Arimoto, J. Math. Chem. 34 (2003) 253–257.
[4] S. Arimoto and K. Fukui, IFC Bulletin (1998) 7–13. (available at http://duke.usask.ca/∼arimoto/)
[5] S. Arimoto, K. Fukui, P. Zizler, K.F. Taylor and P.G. Mezey, Int. J. Quant. Chem. 74 (1999) 633.
[6] S. Arimoto, M. Spivakovsky, H. Ohno, P. Zizler, K.F. Taylor, T. Yamabe, and P.G. Mezey, Int. J. Quant. Chem. 84 (2001) 389.
[7] S. Arimoto, M. Spivakovsky, H. Ohno, P. Zizler, R.A. Zuidwijk, K.F. Taylor, T. Yamabe, and P.G. Mezey, Int. J. Quant. Chem. 97 (2004) 765.
[8] R.J. Walker, *Algebraic Curves* (Princeton University Press, Princeton, 1950).
[9] P.A. Griffiths, Introduction to Algebraic Curves (American Mathematical Society, Providence, 1989).
[10] J.B. Conway, *Functions of One Complex Variable* (Springer, New York, 1973).
[11] S. Arimoto and M. Spivakovsky, J. Math. Chem. 13 (1993) 217.
[12] S. Arimoto and G.G. Hall, Int. J. Quantum Chem. 41 (1992) 613.
[13] S. Arimoto and K.F. Taylor, J. Math. Chem. 13 (1993) 265.