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The Functional Delta Existence Theorem and the reduction of a proof of the Fukui conjecture to that of the Special Functional Asymptotic Linearity Theorem

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Dedicated to the memory of the late Professors Kenichi Fukui and Haruo Shingu

This article establishes a fundamental existence theorem, called the Functional Delta Existence Theorem (DET), which is significant for a new development in the repeat space theory (RST) and also for elucidating an empirical asymptotic principle from experimental chemistry. By using the Functional DET, we reduce a proof of the Fukui conjecture to that of a special and simpler version of the Asymptotic Linearity Theorem (ALT). This reduction provides a basis for the forthcoming series of articles entitled "Proof of the Fukui conjecture via resolution of singularities and related methods". A proof of the Functional DET is given here in a unifying manner so that an investigative link is formed among: (i) fundamental methodology in the RST, which is referred to as the approach via the aspect of form and general topology, (ii) frontier electron theory of reactivity indices, and (iii) the Shingu–Fujimoto empirical asymptotic principle for long chain molecules.

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

1. Introduction

This article is a direct continuation of the preceding article [1]. The present and preceding papers form a basis for the first [2] and subsequent parts of the series entitled "Proof of the Fukui conjecture via resolution of singularities and related methods", which are to appear in this journal. We retain all the notation given in [1], and recall the fact that the validity of the following conjecture immediately follows from what we called the Functional Asymptotic Linearity Theorem (ALT), which was proved in [1] and is reproduced in section 2.

The Fukui conjecture. 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

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eigenvalues 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 $N \to \infty$.

We thus have the following logical implication:

$$\text{Functional ALT} \quad \Rightarrow \quad \text{the Fukui conjecture}.$$

The main objective of this article is to reduce a proof of the Fukui conjecture to what we call the Special Functional Asymptotic Linearity Theorem, by establishing the following logical implication:

$$\text{Special Functional ALT} \quad \Rightarrow \quad \text{Functional ALT}.$$

After formulating the problem in section 2, we attain this objective in sections 3 and 4 by establishing a fundamental existence theorem called the Functional Delta Existence Theorem (DET). This theorem is significant for the new development in the repeat space theory (RST), namely for the above mentioned forthcoming series of articles related to the Fukui conjecture, and also for elucidating an empirical asymptotic principle from experimental chemistry [3,4], which together with the notion of logical interface π is expounded in section 5.

In parts VI and VII [5,6] of the series of articles entitled, "Structural analysis of certain linear operators representing chemical network systems via the existence and uniqueness theorems of spectral resolution", a mathematical and methodical link has been established between

(i) fundamental methodology in the RST, which is referred to as the approach via the aspect of form and general topology, and

(ii) frontier electron theory of reactivity indices [7–12].

The methodology (i) originates from [13] and part of it was formulated into unifying practical theorems, theorems 4.3 and 4.4, in the preceding article [1] so that they are applicable also to the topological closure extension procedures in [5,6] and in the earlier papers [14,15].

Our main theorem in the present paper, the Functional DET, is also established by using the above methodology (i) and [1, theorem 4.3], so that an investigative link is formed among (i), (ii), and

(iii) the Shingu–Fujimoto empirical asymptotic principle for long chain molecules [3,4] (cf. section 5).

2. Formulation of the problem

Throughout, we retain the notation and conventions in [1]. (The reader is asked to review all the notation, conventions, and main results therein.) Recall the main theorem established in [1], which immediately implies the validity of the Fukui conjecture:

Theorem 2.1 (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

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.1}$$

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

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

$$X_r(q) = X_{\#\alpha}(q) \dot{+} X_\beta(q). \tag{2.2}$$

Since,

$$X_{\#\alpha}(q) \subset X_r(q), \tag{2.3}$$

the following theorem, which we call the Special Functional ALT, evidently follows from the above theorem.

Theorem 2.2 (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

$$\operatorname{Tr} \varphi(A_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.4}$$

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

Our problem is as follows:

Problem I. Is it possible to reduce the proof of the Functional ALT to that of the Special Functional ALT, so that we have a new way of proving the Fukui conjecture via the following logical implications:

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

Due to the structural simplicity of $X_{\#\alpha}(q)$ compared with $X_r(q)$, if this problem is solved affirmatively and the above new route of proving the Fukui conjecture is established, one can see the crux of the phenomena of the asymptotic linearity in the RST more efficiently and deeply than before.

In section 3, we provide the affirmative solution to the above problem by our main theorem, the Functional DET, and by the following theorem established in [1].

Theorem 2.3 (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)

$$\bigcup_{0\leqslant\theta\leqslant 2\pi} \sigma\big(F(\theta)\big) = \overline{\bigcup_{N\geqslant 1} \sigma(A_N)}. \tag{2.5}$$

(ii)

$$\bigcup_{0\leqslant\theta\leqslant 2\pi} \sigma\big(F(\theta)\big) \subset \overline{\bigcup_{N\geqslant 1} \sigma(M_N)}. \tag{2.6}$$

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

3. Solution of the problem by the Functional Delta Existence Theorem and the Compatibility Theorem

We begin this section by formulating our main theorem:

Theorem 3.1 (Functional DET, $X_r(q)$ version). Let $\{M_N\}, \{M'_N\} \in X_r(q)$ be fixed repeat sequences with $\{M_N\} - \{M'_N\} \in X_\beta(q)$. Let I be a fixed closed interval compatible with $\{M_N\}$ and $\{M'_N\}$. Define the sequence of linear functionals $\Delta_N : AC(I) \to \mathbb{R}$ by

$$\Delta_N(\varphi) = \operatorname{Tr}\varphi(M_N) - \operatorname{Tr}\varphi\big(M'_N\big). \tag{3.1}$$

Then, there exists a functional $\Delta \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ such that

$$\Delta_N(\varphi) = \Delta(\varphi) + o(1) \tag{3.2}$$

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

Assuming the validity of the above theorem 3.1, which shall be proved in section 4, we can state

Proof of theorem 2.1 (by means of the reduction to the Special Functional ALT, answer to problem I). Let $\{A_N\} \in X_{\#\alpha}(q)$ be the standard α sequence such that

$$\{M_N\} - \{A_N\} \in X_\beta(q). \tag{3.3}$$

Express $\operatorname{Tr}\varphi(M_N)$ as follows:

$$\operatorname{Tr}\varphi(M_N) = \operatorname{Tr}\varphi(A_N) + \big(\operatorname{Tr}\varphi(M_N) - \operatorname{Tr}\varphi(A_N)\big). \tag{3.4}$$

Using the Functional DET and the Compatibility Theorem reproduced at the end of section 2, one easily sees that the proof of the Functional ALT is reduced to that of the Special Functional ALT. □

4. Proof of the Functional Delta Existence Theorem

Before proving the Functional DET, we recall the following theorems 4.1–4.4 whose proofs were given in [1]. Note that theorem 4.4 was proved in [1] by using the unifying fundamental methodology of the RST – the approach via the aspect of form and general topology. (Theorems 4.1 and 4.2 correspond to the approach via the aspect of form and theorem 4.3 corresponds to the approach via the aspect of general topology; theorem 4.4 was proved by using theorems 4.1, 4.2, and 4.3.)

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

$$\operatorname{Tr}\varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) \tag{4.1}$$

for all $N \gg 0$.

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

$$\big\{\varphi(M_N)\big\} \in X_r(q). \tag{4.2}$$

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 $o_T = \{\varnothing, \{\boldsymbol{F}\}, \{\boldsymbol{T}, \boldsymbol{F}\}\}$. Consider the mapping $\pi : X \to \boldsymbol{L}$ defined by

$$\pi(\varphi) = \begin{cases} \boldsymbol{T} & \text{if } \{\tau_N(\varphi)\} \text{ is convergent,} \\ \boldsymbol{F} & \text{if } \{\tau_N(\varphi)\} \text{ is not convergent.} \end{cases} \tag{4.3}$$

Suppose that

$$\sup\big\{\|\tau_N\|\colon N \geqslant 1\big\} < \infty. \tag{4.4}$$

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: $\tau \in \boldsymbol{B}(X, \mathscr{B})$.

Remark 4.1. The proof of the above theorem 4.3 is based on theorem 4.4 in [1], which we do not reproduce here, but corresponds to the approach via the aspect of general topology and provides important logical insights into the assertion of the above theorem 4.3.

Theorem 4.4 (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

$$\frac{\operatorname{Tr} \varphi(M_N)}{N} = \alpha(\varphi) + o(1) \tag{4.5}$$

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

At this moment, we recommend the reader to briefly review the proof process of the above theorem 4.4 in [1]. We prove the Functional DET, in an analogous way, namely by using theorem 4.3 and the subsequent theorems 4.1* and 4.2* which are analogous to the above theorems 4.1 and 4.2, respectively.

Theorem 4.1* (Polynomial DET, $X_r(q)$ version). Let $\{M_N\}, \{M'_N\} \in X_r(q)$ be fixed repeat sequences with $\{M_N\} - \{M'_N\} \in X_\beta(q)$. Let I be a fixed closed interval compatible with $\{M_N\}$ and $\{M'_N\}$. Then, for any $\varphi \in P(I)$ there exists a $\Delta(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) - \operatorname{Tr} \varphi(M'_N) = \Delta(\varphi) \tag{4.6}$$

for all $N \gg 0$.

Proof. The conclusion follows immediately from the definition of $X_\beta(q)$ and theorem 4.2* below. □

Theorem 4.2*. The notation and assumptions being as in theorem 4.1*, assume that $\varphi \in P(I)$. We have

$$\{\varphi(M_N)\} - \{\varphi(M'_N)\} \in X_\beta(q). \tag{4.7}$$

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

$$\varphi(t) = c_0 t^0 + \cdots + c_n t^n, \tag{4.8}$$

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

$$\begin{aligned} \{\varphi(M_N)\} - \{\varphi(M'_N)\} &= \{c_0 M_N^0 + \cdots + c_n M_N^n\} - \{c_0 M_N'^0 + \cdots + c_n M_N'^n\} \\ &= \{c_1 M_N^1 + \cdots + c_n M_N^n\} - \{c_1 M_N'^1 + \cdots + c_n M_N'^n\}. \end{aligned} \tag{4.9}$$

Since $X_\beta(q)$ is a linear space, to show that (4.7) is true, we have only to verify that $m \in \mathbb{Z}^+$ implies that

$$\{M_N^m\} - \{M_N'^m\} \in X_\beta(q). \tag{4.10}$$

But, (4.10) can be easily proved by induction on m, bearing in mind the fact that if $\{K_N\}, \{K'_N\}, \{L_N\}, \{L'_N\} \in X_r(q)$, $\{K_N\} - \{K'_N\} \in X_\beta(q)$, and $\{L_N\} - \{L'_N\} \in X_\beta(q)$, then

$$\{K_N\} \circ \{L_N\} - \left\{K'_N\right\} \circ \left\{L'_N\right\} \in X_\beta(q), \tag{4.11}$$

where $\circ$ denotes the Jordan product operation defined by

$$\{K_N\} \circ \{L_N\} = \left\{\frac{1}{2}(K_N L_N + L_N K_N)\right\} \tag{4.12}$$

(cf. [16] for details). □

We need some more preparation for a proof of the Functional DET.

Theorem 4.5. The notation and assumptions being as in theorem 3.1, there exist $r, n \in \mathbb{Z}^+$ such that

$$\left|\Delta_N(\varphi)\right| \leqslant r V_I(\varphi) \tag{4.13}$$

for all $\varphi \in AC(I)$ and $N > n$.

Proof. We first recall that

$$AC(I) \subset BV(I), \tag{4.14}$$

(cf. [1, section 3]) and the following lemma from article [1]:

Lemma 7.1 [1]. Let $n \in \mathbb{Z}^+$ with $n \geqslant 2$, let $K = \{k_1, k_2, \ldots, k_r\}$ be a subset of $\{1, 2, \ldots, n\}$ consisting of r distinct elements ($1 \leqslant r < n$), and let $L = \{1, 2, \ldots, n\} \backslash K$. 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

$$\left(M - M'\right)_{ij} = 0 \tag{4.15}$$

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

$$\left|\operatorname{Tr}\varphi(M) - \operatorname{Tr}\varphi\left(M'\right)\right| \leqslant r V_I(\varphi) \tag{4.16}$$

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

By the definition of $X_\beta(q)$, for all $N \gg 0$, $M_N - M'_N$ has the following form:

$$M_N - M'_N = \begin{pmatrix} W_1 & & W_2 \\ & \mathbf{0} & \\ W_3 & & W_4 \end{pmatrix}, \tag{4.17}$$

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. Hence, for all $N \gg 0$, we may apply [1, lemma 7.1] to get the conclusion. □

Theorem 4.6. The notation and assumptions being as in theorem 3.1, we have

(i) For all $N \in \mathbb{Z}^+$,

$$\Delta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R}). \tag{4.18}$$

(ii)

$$\sup\left\{\|\Delta_N\|:\ N \geqslant 1\right\} < \infty. \tag{4.19}$$

Proof. (i) Note that the following relations

$$\begin{aligned}\left|\Delta_N(\varphi)\right| &\leqslant \left|\operatorname{Tr}\varphi(M_N)\right| + \left|\operatorname{Tr}\varphi\left(M_N'\right)\right| \\ &\leqslant 2qN\left(\sup\left\{\left|\varphi(t)\right|:\ t \in I\right\}\right) \\ &\leqslant 2qN\left(\sup\left\{\left|\varphi(t)\right|:\ t \in I\right\} + V_I(\varphi)\right) = 2qN\|\varphi\|\end{aligned} \tag{4.20}$$

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

(ii) By theorem 4.5, there exist $r, n \in \mathbb{Z}^+$ such that

$$\left|\Delta_N(\varphi)\right| \leqslant rV_I(\varphi) \leqslant r\|\varphi\| \tag{4.21}$$

for all $\varphi \in AC(I)$ and $N > n$. By (4.20) and (4.21), (ii) is true. □

Now we are ready to give a proof of our main theorem.

Proof of theorem 3.1 (*Functional DET*). First, recall from theorem 4.6(i) that $\Delta_N \in AC(I)^* = \boldsymbol{B}(AC(I), \mathbb{R})$ for all $N \in \mathbb{Z}^+$. Second, recall the fact that $P(I)$ is a dense subset of $AC(I)$:

$$\overline{P(I)} = AC(I) \tag{4.22}$$

(cf. [1,17]).

It is easy to check that

(d1) for all $\varphi \in P(I)$, $\lim_{N\to\infty} \Delta_N(\varphi)$ exists in $\mathbb{R}$,

(d2) $\sup\{\|\Delta_N\|:\ N \geqslant 1\} < \infty$,

(d3) for all $\varphi \in AC(I)$, $\lim_{N\to\infty} \Delta_N(\varphi)$ exists in $\mathbb{R}$,

(d4) $\Delta : AC(I) \to \mathbb{R}$ defined by

$$\Delta(\varphi) = \lim_{N\to\infty} \Delta_N(\varphi) \tag{4.23}$$

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

In fact, (d1) follows from theorem 4.1*, (d2) from theorem 4.6(ii). Note that (4.22), (d1), (d2), and theorem 4.3(iii) imply (d3) and (d4). From (d4) the conclusion follows. □

5. The Functional Delta Existence Theorem, an empirical asymptotic principle from experimental chemistry, and logical interface π

Systematic asymptotic analyses on thermodynamic and spectroscopic data were undertaken in [3,4] for a study of correlation between molecular structure and energies in hydrocarbons. The formation of the Functional DET has been highly motivated by Haruo Shingu and Takehiko Fujimoto's empirical asymptotic principle called "the long chain criteria principle", which was initially derived from the observation on "the constancy of isomeric variations of the same kind in the molecular energies of the long chain paraffin hydrocarbons" (cf. [3,4]).

It is convenient at this moment of reflection on this principle to introduce the following definitions in conjunction with theorem 4.3.

Definitions 5.1. Let $\boldsymbol{L}$ denote the topological space with the underlying set $\{\boldsymbol{T}, \boldsymbol{F}\}$ and the system of open sets $o_T = \{\varnothing, \{\boldsymbol{F}\}, \{\boldsymbol{T}, \boldsymbol{F}\}\}$. The topological space $\boldsymbol{L}$ is called the *logical space*. Let $X, X_1, \ldots, X_n$ be topological spaces, let $\pi : X \to \boldsymbol{L}$ be a continuous mapping, let $\rho_1 : X \to X_1, \ldots, \rho_n : X_{n-1} \to X_n$, and $\rho_{n+1} : X_n \to \boldsymbol{L}$ be continuous mappings such that the following diagram

$$
\begin{array}{ccccccccc}
X & & & \xrightarrow{\quad\quad\quad\pi\quad\quad\quad} & & & & & \boldsymbol{L} \\
\Big\downarrow{\scriptstyle \rho_1} & & & & & & & & \Big\uparrow{\scriptstyle \rho_{n+1}} \\
X_1 & \xrightarrow[\rho_2]{} & X_2 & \xrightarrow[\rho_3]{} & \cdots & \longrightarrow & X_{n-1} & \xrightarrow[\rho_n]{} & X_n
\end{array}
$$

is commutative, i.e., such that

$$\pi = \rho_{n+1} \circ \cdots \circ \rho_1. \tag{5.1}$$

The mapping π is called a *logical interface* on X. Each ρ_i, $1 \leqslant i \leqslant n+1$, is called a *component* of π. Equality (5.1) is called a *component analysis* of π.

We note that the empirical asymptotic principle for the zero-point energy and thermodynamic quantities of molecules having many identical moieties can be mathematically elucidated by using the Functional DET and component analyses of logical interface π, whose definition was given above in conjunction with theorem 4.3. The application of the Functional DET along these lines needs some preparation and will be published elsewhere.

The author recalls with pleasure discussions on the additivity problems of organic compounds with the late Professors Kenichi Fukui and Haruo Shingu, especially those valuable discussions on the dialectic and mutually beneficial interplay between theory and experiment, which later lead the author to form the following:

(i) the approach using diagrams of arrows [5,6,14,15,18,19] in the RST,

(ii) the notion of logical interface π which assists in bridging the gap between theoretical and experimental languages in chemistry, and

(iii) the idea and applications of component analyses of π.

It should be noted that the above (i)–(iii) have been successfully used not only as research tools in the RST but as communication and/or pedagogical devices for those who are unfamiliar with the physico-chemical applications of the RST, which aims to assist in cultivating the fertile interdisciplinary research field between chemistry and modern mathematics.

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