Aspects of form and general topology: Alpha Space Asymptotic Linearity Theorem and the spectral symmetry of alternants

Shigeru Arimoto*

Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 0W0

and

Keith Taylor

Department of Mathematics, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 0W0

Received 7 November 1991; in final form 22 July 1992

A theoretical device and a technique have been developed by which one can study, in a unifying manner, additive properties of hydrocarbons and the symmetric property of the spectrum of alternants. By using functionals introduced in the approach via the aspects of form and general topology, a special version of the Asymptotic Linearity Theorem (for the study of additivity problems of the zero-point vibrational energy of hydrocarbons and the total pi-electron energy of alternants) has been obtained in parallel with a derivation of the spectral symmetry of alternants.

1. Introduction

Special magnitudes of universal constants and specific forms of functions manifest themselves in the expressions of natural laws. Nevertheless, it is sometimes legitimate and meaningful to embed fixed constants or functions into a broader context and make them change. For example, one can regard the Planck constant as a variable and let it tend to zero so that one recognizes classical mechanics to be a limit of quantum mechanics.

In the study of additivity problems of the zero-point vibrational energies (ZPVEs), it was a significant step to embed the square root function in a formula $E = (\hbar/2) \sqrt{k/m}$ into a functional space endowed with a suitable topology, allowing the function to change in the space.

^{*}On leave from: Institute for Fundamental Chemistry, 34-4 Nishihiraki-cho, Takano, Sakyo-ku, Kyoto 606, Japan.

New approaches using the aspects of form and general topology [1-5] based on the above process of embedding a fixed function into a functional space have made it possible to unite the zero-point vibrational energy additivity problem [1-14]with that of the total pi-electron energies (TPEEs) of alternant hydrocarbons [2-5, 15-25], which have long been investigated as separate problems.

The present paper proceeds along the lines of these approaches and provides a special version of the Asymptotic Linearity Theorem (for the study of additivity problems of the ZPVE of hydrocarbons and the TPEE of alternant hydrocarbons), and derives the spectral symmetry of alternants using functional α introduced in ref. [2].

The symmetry of the spectrum of adjacency matrices associated with the alternants is well known, and it can be understood by the Coulson-Rushbrooke Theorem (see a recent review article [26] on this theorem and the references therein).

The idea of the striking connection between functional α and the spectral symmetry naturally follows from closer observation of the special version of the Asymptotic Linearity Theorem given in section 2.

2. Alpha Space Asymptotic Linearity Theorem

Let X(q) (with a fixed $q \in \mathbb{Z}^+$) denote the real linear space of all matrix sequences whose Nth term M_N is an arbitrary $qN \times qN$ real symmetric matrix equipped with the linear operations defined by

$$\{M_N\} + \{M'_N\} = \{M_N + M'_N\}, \qquad (2.1)$$

$$k\{M_N\} = \{kM_N\},$$
 (2.2)

 $N \in \mathbb{Z}^+$ [1,2,4,5]. In the space X(q), operations \circ , $\hat{\psi}$, and $(\cdot)^n$ were also defined:

$$\{M_N\} \circ \{M'_N\} = \left\{ \frac{1}{2} (M_N M'_N + M'_N M_N) \right\},$$
(2.3)

$$\hat{\psi}\{M_N\} = \{c_0 M_N^0 + c_1 M_N^1 + \ldots + c_n M_N^n\}, \qquad (2.4)$$

$$\{M_N\}^n = \{M_N^n\}, (2.5)$$

and they were called, respectively, the Jordan product operation, the polynomial operation associated with polynomial $\psi = c_0 t^0 + c_1 t^1 + \ldots + c_n t^n$ with real coefficients, and the *n*th power operation, $n \in \mathbb{Z}_0^+$.

Let the repeat space $X_r(q)$, alpha space $X_{\alpha}(q)$, and beta space $X_{\beta}(q)$ with block-size q be defined as in refs. [1,2,4,5].

Theorem 1 given below, which was obtained by an approach using the aspect of form, played an important role in establishing fundamental theorems for the study of the additivity problems of the ZPVEs and TPEEs:

- (i) the α Existence Theorem [2],
- (ii) the α Independence Theorem [2],
- (iii) the α Representation Theorem [4],
- (iv) the Asymptotic Linearity Theorem [5].

The Alpha Space Asymptotic Linearity Theorem $(X_{\alpha}ALT)$, which we shall establish in this section, is a specialized version of the (iv) above, the Asymptotic Linearity Theorem (ALT). We shall use theorem 1 for the proof of the $X_{\alpha}ALT$.

THEOREM 1

Let $\{r_N\}$, $\{r'_N\} \in X_r(q)$, $\{a_N\}$, $\{a'_N\} \in X_{\alpha}(q)$ and $\{b_N\}$, $\{b'_N\} \in X_{\beta}(q)$ be arbitrary, let k, k' denote any real numbers, and let $\psi = c_0 t^0 + c_1 t^1 + \ldots + c_n t^n$ denote any polynomial with real coefficients. Then the following are true:

(i)
$$k\{r_N\} + k'\{r'_N\} \in X_r(q),$$
 (2.6)

$$\{r_N\} \circ \{r'_N\} \qquad \in X_r(q), \tag{2.7}$$

$$\hat{\psi}(\{r_N\}) \in X_r(q), \tag{2.8}$$

(ii)
$$k\{a_N\} + k'(a'_N) \in X_{\alpha}(q),$$
 (2.9)

$$\{a_N\} \circ \{a'_N\} \qquad \in X_{\alpha}(q), \tag{2.10}$$

$$\hat{\psi}(\{a_N\}) \quad \in X_{\alpha}(q), \tag{2.11}$$

(iii)
$$k\{b_N\} + k'\{b'_N\} \in X_\beta(q),$$
 (2.12)

$$\{r_N\} \circ \{b_N\} = \{b_N\} \circ \{r_N\} \quad \in X_{\beta}(q), \tag{2.13}$$

if
$$\{r_N\} - \{r'_N\}$$
 $\in X_\beta(q)$ holds,
then $\hat{\psi}(\{r_N\}) - \hat{\psi}(\{r'_N\})$ $\in X_\beta(q)$ is true. (2.14)

Remark

Relations (2.8) and (2.11), respectively, imply that $X_r(q)$ and $X_{\alpha}(q)$ are closed under any polynomial operation. Note that $X_{\beta}(q)$ is not always closed under polynomial operation (e.g. if $\psi = 1 + t$, then $\hat{\psi}(\{b_N\}) \notin X_{\beta}(q)$). However, $X_r(q), X_{\alpha}(q)$, and $X_{\beta}(q)$ are all closed under the linear operations, i.e. they are linear subspaces of X(q).

Now recall the ZPVE of a linear chain $Ch_N^{"}$ with cyclic ends which consists of N particles of mass 1 at separation 1 with nearest-neighbour interaction whose

force constant is 1 [2]. Let $\{M_N\}$ denote an element of the alpha space $X_{\alpha}(1)$ with block-size 1 such that M_N is an $N \times N$ matrix given by

for all $N \ge 2$.

Put $\hbar/2 = 1$ for simplicity. Then the ZPVE E_N of the linear chain Ch_N'' is expressed by

$$E_N = \sum_{i=1}^N \varphi(\lambda_i(M_N)) = \operatorname{Tr} \varphi(M_N), \qquad (2.16)$$

where $\lambda_i(M_N)$ denotes the *i*th eigenvalue of M_N , the φ denotes the function $\varphi: t \mapsto |t|^{1/2}$ defined on a fixed closed interval *I* compatible with $\{M_N\}$ (see refs. [1,2,4,5] for the definition of a function of a matrix and the compatibility of *I*).

The eigenvalues of M_N with $N \ge 2$ can be obtained explicitly in terms of the sine function. Using a simple formula for the sum of the trigonometric functions, one obtains an analytic expression for E_N :

$$E_N = 2 \cot(\pi/2N).$$
 (2.17)

Since $\cot \theta = 1/\theta - \frac{1}{3}\theta$ + (higher-order terms) for $\theta \in (0, \pi)$, we can express

$$E_N = \alpha N + o(1) \tag{2.18}$$

as $N \to \infty$, where $\alpha = 4/\pi$. This shows that E_N has an asymptotic line whose intercept vanishes.

The Asymptotic Linearity Theorem can be applied to the above system since $\{M_N\} \in X_{\alpha}(1) \subset X_r(1)$, and one can predict that E_N has an asymptotic line $\alpha N + \beta$, where $\alpha, \beta \in \mathbb{R}$. However, from the Asymptotic Linearity Theorem it does not follow that the intercept β should vanish.

By straightforward calculations of matrix multiplications, for large enough N's, we see that the second power of M_N is given by an $N \times N$ matrix:

Calculating M_N^k further (k = 3, 4, ...), one can inductively find that M_N^k possesses a repeating pattern along the diagonal and that $\operatorname{Tr} M_N^k = \alpha_k N$ for all $N \gg 0$ (for all N greater than some given positive integer), where α_k is a real number dependent on k ($\alpha_0 = 1$, $\alpha_1 = 2$, $\alpha_2 = 6$, $\alpha_3 = 20$, ...).

Hence, given a polynomial function φ with $\varphi(t) = c_0 t^0 + c_1 t^1 + \ldots + c_n t^n$, one can conjecture that $\operatorname{Tr} \varphi(M_N) = (\sum_{k=1}^n c_k \alpha_k) N$ for all $N \gg 0$ and that for any polynomial function φ defined on *I*, $\operatorname{Tr} \varphi(M_N)$ has an asymptotic line which goes through the origin. In fact, this can be verified generally by theorem 2 given below.

Henceforth, by P(I) we shall denote the set of all polynomial functions with real coefficients defined on a closed interval I.

THEOREM 2 (X_{α} PALT)

Let $\{M_N\} \in X_{\alpha}(q)$ be a fixed α sequence, let *I* be a fixed closed interval compatible with $\{M_N\}$. Then for any element $\varphi \in P(I)$, there exists an $\alpha(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N \tag{2.20}$$

for all $N \gg 0$.

Proof

Let φ be such that

$$\varphi(t) = c_0 t^0 + c_1 t^1 + \ldots + c_n t^n, \qquad (2.21)$$

 $t \in I$. Then we have

$$\varphi(M_N) = c_0 M_N^0 + c_1 M_N^1 + \ldots + c_n M_N^n.$$
(2.22)

Recall the fact that the α space with block-size q, $X_{\alpha}(q)$, is closed under any polynomial operation (cf. theorem 1). By this closure property and (2.22), we easily see that

$$\{\varphi(M_N)\} \in X_{\alpha}(q). \tag{2.23}$$

On the other hand, by the definition of $X_{\alpha}(q)$, for all $N \gg 0$, the $qN \times qN$ matrix $\varphi(M_N)$ possesses, along the diagonal, N repeating $q \times q$ submatrices $Q_0(\varphi)$. Putting

$$\alpha(\varphi) = \operatorname{Tr} Q_0(\varphi), \tag{2.24}$$

the conclusion follows.

We shall call the above theorem the α Space Polynomial Asymptotic Linearity Theorem (X_{α} PALT).

As we demonstrated the Asymptotic Linearity Theorem (ALT) using the Polynomial Asymptotic Linearity Theorem (PALT) [5], we can derive the α Space Asymptotic Linearity Theorem (X_{α} ALT) from the α Space Polynomial Asymptotic Linearity Theorem (X_{α} PALT), which we shall do below.

Let CBV(I) denote the real normed space of all real-valued continuous functions of bounded variation defined on a closed interval I = [a, b] $(a, b \in \mathbb{R}, a < b)$ equipped with the norm given by

$$\|\varphi\| = \sup_{t \in I} |\varphi(t)| + V_I(\varphi),$$
(2.25)

where $V_I(\varphi)$ denotes the total variation of φ on *I*. Then the closure \overline{P} of P = P(I) in the normed space CBV(*I*) forms a closed subspace of CBV(*I*) and contains all the functions $t \mapsto |t|^{\xi} (\xi > 0)$ defined on *I*.

Now we are ready to state and prove

THEOREM 3 (X_{α} ALT)

Let $\{M_N\} \in X_{\alpha}(q)$ be a fixed α sequence, let *I* be a fixed closed interval compatible with $\{M_N\}$. Then, for any element $\varphi \in \overline{P}$ in the normed space CBV(*I*), there exists an $\alpha(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + o(1) \tag{2.26}$$

as $N \to \infty$.

Proof

Recalling the fact that $X_{\alpha}(q) \subset X_r(q)$, we can apply the Asymptotic Linearity Theorem to conclude that, for any $\varphi \in \overline{P}$, there exist $\alpha(\varphi)$, $\beta(\varphi) \in \mathbb{R}$ such that

$$\operatorname{Tr} \varphi(M_N) = \alpha(\varphi)N + \beta(\varphi) + o(1) \tag{2.27}$$

as $N \to \infty$. Here, one can regard $\alpha(\varphi)$ as a value of a continuous functional α : $C(I) \to \mathbb{R}$ defined by

$$\alpha(\varphi) = \lim_{N \to \infty} [\operatorname{Tr} \varphi(M_N)] / N, \qquad (2.28)$$

$$\beta(\varphi) = \lim_{N \to \infty} \beta_N(\varphi), \tag{2.29}$$

where

$$\beta_N(\varphi) = \operatorname{Tr} \varphi(M_N) - \alpha(\varphi)N. \tag{2.30}$$

See section 3 for the continuity of α . In ref. [5], it has been proved that functionals $\overline{\beta}$, β : CBV(I) $\rightarrow \mathbb{R}$ defined by

$$\overline{\beta}(\varphi) = \limsup_{N \to \infty} \beta_N(\varphi), \tag{2.31}$$

$$\underline{\beta}(\varphi) = \liminf_{N \to \infty} \beta_N(\varphi) \tag{2.32}$$

are both continuous. Thus, we easily see that β is a continuous functional.

By theorem 1, β vanishes on the subset P,

$$\beta(P) = \{0\}. \tag{2.33}$$

However, β is continuous so that we have $\beta(\overline{P}) \subset \overline{\beta(P)}$ and

$$\beta(\overline{P}) \subset \overline{\{0\}} = \{0\}. \tag{2.34}$$

On the other hand, it is clear that

$$\beta(\overline{P}) \supset \beta(P) = \{0\}. \tag{2.35}$$

Therefore, β vanishes on the closure \overline{P} of P,

$$\beta(\overline{P}) = \{0\},\tag{2.36}$$

from which the conclusion follows immediately.

Note that if S is an arbitrary subset of the domain of β , then (i) implies (ii),

(i)
$$\beta(S) = \{0\},$$
 (2.37)

(ii)
$$\beta(\overline{S}) = \{0\}.$$
 (2.38)

Likewise, if S is any subset of C(I), $\alpha(S) = \{0\}$ implies $\alpha(\overline{S}) = \{0\}$. We shall use this property of α to derive the spectral symmetry of alternants in section 3.

Remark on theorem 3 (X_{α} ALT)

We have proved theorem 3 ($X_{\alpha}ALT$) by using the ALT (the Asymptotic Linearity Theorem), theorem 2 (the α Space Polynomial Asymptotic Linearity

П

Theorem), and the continuity of the functional β defined by (2.29). It should be remarked that the $X_{\alpha}ALT$ and the ALT involve the same broad function space $\overline{P} \subset CVB(I)$, from which the strength of these two theorems arises.

The reader is referred to refs. [1,2] and [4] for an explanation of the usual approaches to the additivity problems. These conventional approaches are not effective for establishing the ALT [1,5] and the X_{α} ALT above, which are formulated in a new and broader context.

3. Alpha functionals and spectral symmetry of alternants

Let C(I) denote the real normed space of all real-valued continuous functions defined on a closed interval I = [a, b] $(a, b \in \mathbb{R}, a < b)$ equipped with the sup norm $\|\cdot\|_{\infty}$ given by

$$\|\varphi\|_{\infty} = \sup_{t \in I} |\varphi(t)|.$$
(3.1)

We note that, since I is compact, the supremum is always achieved, so sup could be replaced by max in the definition of $||\varphi||_{\infty}$.

Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, let *I* be a fixed closed interval compatible with $\{M_N\}$. The functional $\alpha: C(I) \to \mathbb{R}$ defined by

$$\alpha(\varphi) = \lim_{N \to \infty} [\operatorname{Tr} \varphi(M_N)] / N$$
(3.2)

is linear and bounded; henceforth, it will be called the "alpha functional of $\{M_N\}$ with domain C(I)". (Note that the functional is well defined by the α Existence Theorem.)

The functional is indeed linear, i.e.

$$\alpha(k_1\varphi_1 + k_2\varphi_2) = k_1\alpha(\varphi_1) + k_2\alpha(\varphi_2)$$
(3.3)

holds for all $\varphi_1, \varphi_2 \in C(I)$ and $k_1, k_2 \in \mathbb{R}$. The validity of this relation follows from the easily verifiable equality

$$(k_1\varphi_1 + k_2\varphi_2)(M_N) = k_1(\varphi_1(M_N)) + k_2(\varphi_2(M_N)),$$
(3.4)

and the linearity of the trace operation and the " $\lim_{N\to\infty}$ ".

The functional is bounded, i.e. there exists a constant $c \in \mathbb{R}$ such that

$$|\alpha(\varphi)| \le c \, \|\varphi\|_{\infty} \tag{3.5}$$

holds for all $\varphi \in C(I)$. This follows immediately from the inequalities

$$|\alpha(\varphi)| \leq \lim_{N \to \infty} \left[\sum_{i=1}^{qN} |\varphi(\lambda_i(M_N))| \right] / N \leq q \|\varphi\|_{\infty}.$$
(3.6)

Hence, we see that α is linear and bounded, thus continuous. We remark that the continuity of α can also be proved by the continuity of the functionals $\overline{\alpha}$, $\underline{\alpha}$: $C(I) \rightarrow \mathbb{R}$ defined by

$$\overline{\alpha}(\varphi) = \limsup_{N \to \infty} [\operatorname{Tr} \varphi(M_N)]/N, \qquad (3.7)$$

$$\underline{\alpha}(\varphi) = \liminf_{N \to \infty} [\operatorname{Tr} \varphi(M_N)]/N, \qquad (3.8)$$

(see ref. [2] for details).

Now we can exactly formulate the statement on α given at the end of section 2.

PROPOSITION 1

Let $\{M_N\} \in X_r(q)$ be a fixed repeat sequence, and let *I* be a fixed closed interval compatible with $\{M_N\}$. Let α be the alpha functional of $\{M_N\}$ with domain C(I), and let *S* be any subset of C(I). Then (i) implies (ii),

(i)
$$\alpha(S) = \{0\},$$
 (3.9)

(ii)
$$\alpha(\overline{S}) = \{0\}.$$
 (3.10)

Proof

By the continuity of α , (ii) follows from (i) by the argument analogous with that in the proof of theorem 3.

We shall use the following proposition to verify the spectral symmetry of alternants.

PROPOSITION 2

Let a > 0 and I = [-a, a]. Let $C_0 = C_0(I)$ denote the closed subset of C(I) of all odd functions and let $P_0 = P_0(I)$ denote the subset of P(I) of all odd polynomial functions. Then (i) implies (ii),

(i) $\alpha(P_0) = \{0\},$ (3.11)

(ii)
$$\alpha(C_{o}) = \{0\}.$$
 (3.12)

Proof

By proposition 1, to prove proposition 2, it is enough to prove the following proposition 3. $\hfill \Box$

PROPOSITION 3

Let P_o , C_o be as in proposition 2. Let $C_e = C_e(I)$ denote the closed subset of C(I) of all even functions and let $P_e = P_e(I)$ denote the subset of P(I) of all even functions. Then $\overline{P_e} = C_e$ and $\overline{P_o} = C_o$, where the upper bar denotes the closure operation in the normed space C(I).

Proof

For any $\varphi \in C(I)$, let φ_e and φ_o denote the even and odd part of φ defined by

$$\varphi_{e}(t) = \frac{1}{2} \left(\varphi(t) + \varphi(-t) \right), \qquad \text{for all } t \in I, \qquad (3.13)$$

$$\varphi_{o}(t) = \frac{1}{2} \left(\varphi(t) - \varphi(-t) \right), \qquad \text{for all } t \in I.$$
(3.14)

Note that $C_e = \{ \varphi \in C(I) : \varphi_e = \varphi \}$ and $C_o = \{ \varphi \in C(I) : \varphi_o = \varphi \}$. The following properties are easy to verify:

(i)
$$\varphi = \varphi_{\rm e} + \varphi_{\rm o}$$
. (3.15)

(ii)
$$\|\varphi_e\|_{\infty} \le \|\varphi\|_{\infty}$$
, (3.16)

$$\|\varphi_0\|_{\infty} \le \|\varphi\|_{\infty} \,. \tag{3.17}$$

(iii)
$$(k_1\varphi_1 + k_2\varphi_2)_e = k_1\varphi_{1e} + k_2\varphi_{2e}$$
, (3.18)

$$(k_1\varphi_1 + k_2\varphi_2)_0 = k_1\varphi_{10} + k_2\varphi_{20}, \qquad (3.19)$$

for all
$$\varphi_1, \varphi_2 \in C(I), k_1, k_2 \in \mathbb{R}$$
.

Now, let $\phi \in C_e$ and $\varepsilon > 0$. The Weierstrass approximation theorem implies that there exists $p \in P$ such that $||\phi - p||_{\infty} < \varepsilon$. The (ii) and (iii) imply that

$$||\phi - p_{e}||_{\infty} = ||(\phi - p)_{e}||_{\infty} \le ||\phi - p||_{\infty} < \varepsilon.$$
(3.20)

Thus, P_e is dense in C_e . Similarly, $\overline{P_o} = C_o$.

Now we shall recall the structure of the repeat space $X_r(q)$ with block-size q. The repeat space $X_r(q)$ can be expressed as a sum of its subspaces, the alpha space $X_{\alpha}(q)$, and the beta space $X_{\beta}(q)$,

$$X_r(q) = X_\alpha(q) + X_\beta(q). \tag{3.21}$$

By theorem 1, we can concisely write out the relationship between subspaces $X_{\alpha}(q)$ and $X_{\beta}(q)$ with respect to the Jordan product operation,

(i)
$$X_{\alpha}(q) \circ X_{\alpha}(q) \subset X_{\alpha}(q),$$
 (3.22)

(ii)
$$X_{\alpha}(q) \circ X_{\beta}(q) \subset X_{\beta}(q),$$
 (3.23)

(iii)
$$X_{\beta}(q) \circ X_{\alpha}(q) \subset X_{\beta}(q),$$
 (3.24)

(iv)
$$X_{\beta}(q) \circ X_{\beta}(q) \subset X_{\beta}(q),$$
 (3.25)

where $X_i(q) \circ X_j(q) = \{a \circ b : a \in X_i(q), b \in X_j(q)\}, i, j = \alpha, \beta$. We define new subspaces of $X_\alpha(q)$ as follows.

Let $X_d(q)$ denote the subspace of $X_\alpha(q)$ of all matrix sequences $\{M_N\} \in X_\alpha(q)$ such that

$$M_N = B - \operatorname{diag}(\underbrace{M_1, M_1, \ldots, M_1}_{N}), \qquad (3.26)$$

 $N \in \mathbb{Z}^+$, where M_1 is a $q \times q$ real symmetric matrix, and B-diag reads "the block diagonal matrix whose diagonal blocks are given by ...".

Let $q_1, q_2 \in \mathbb{Z}^+$, and $q = q_1 + q_2$. We shall also define two subspaces $X_d^+(q_1, q_2)$ and $X_d^-(q_1, q_2)$ of $X_d(q)$ as follows.

The subspace $X_d^+(q_1, q_2)$ of $X_d(q)$ is defined to be the set of all matrix sequences $\{M_N\} \in X_d(q)$ such that M_N is given by (3.26) and that

$$M_1 = \begin{pmatrix} W_{11} & \text{zeros} \\ \hline \text{zeros} & W_{22} \end{pmatrix},$$
(3.27)

where W_{11} denotes a $q_1 \times q_1$ real symmetric matrix and W_{22} denotes a $q_2 \times q_2$ real symmetric matrix.

The subspace $X_d^-(q_1, q_2)$ of $X_d(q)$ is defined to be the set of all matrix sequences $\{M_N\} \in X_d(q)$ such that M_N is given by (3.26) and that

$$M_1 = \left(\frac{\text{zeros} | W_{12}}{W_{21} | \text{zeros}}\right), \tag{3.28}$$

where W_{12} denotes a $q_1 \times q_2$ real matrix and W_{21} denotes a $q_2 \times q_1$ real matrix. (Note that $W_{12}^T = W_{21}$ by the symmetry of $M_{1.}$)

We shall call $X_d(q)$, $X_d^+(q_1, q_2)$ and $X_d^-(q_1, q_2)$, respectively, the diagonal space with block-size q, plus diagonal space with block-size (q_1, q_2) , and minus diagonal space with block-size (q_1, q_2) . We shall also call each element of $X_d(q)$, $X_d^+(q_1, q_2)$ and $X_d^-(q_1, q_2)$, respectively, a diagonal sequence, a plus diagonal sequence, and a minus diagonal sequence. It is easy to see that $X_d(q)$, with $q = q_1 + q_2$ can be expressed as a sum of its subspaces $X_d^+(q_1, q_2)$ and $X_d^-(q_1, q_2)$,

$$X_d(q) = X_d^+(q_1, q_2) + X_d^-(q_1, q_2).$$
(3.29)

Let us pay attention to the relationship between the subspaces $X_d^+(q_1, q_2)$ and $X_d^-(q_1, q_2)$ with respect to the Jordan product operation.

THEOREM 4

260

The following statements are true for all $q_1, q_2 \in \mathbb{Z}^+$:

(i)
$$X_d^+(q_1, q_2) \circ X_d^+(q_1, q_2) \subset X_d^+(q_1, q_2),$$
 (3.30)

(ii)
$$X_d^+(q_1, q_2) \circ X_d^-(q_1, q_2) \subset X_d^-(q_1, q_2),$$
 (3.31)

(iii)
$$X_d^-(q_1, q_2) \circ X_d^+(q_1, q_2) \subset X_d^-(q_1, q_2),$$
 (3.32)

(iv)
$$X_d^-(q_1, q_2) \circ X_d^-(q_1, q_2) \subset X_d^+(q_1, q_2).$$
 (3.33)

Proof

By the definitions of $X_d^+(q_1, q_2)$, $X_d^-(q_1, q_2)$, and the Jordan product operation, the validity of each statement follows from the fundamental formulae for blockwise multiplication and addition of block matrices.

THEOREM 5

The minus diagonal space $X_d^-(q_1, q_2)$ with block-size (q_1, q_2) is closed under any odd polynomial operation.

Proof

Let $\{M_N\} \in X_d^-(q_1, q_2)$ be arbitrary and let $\psi = c_1 t^1 + c_3 t^3 + \ldots + c_{2n+1} t^{2n+1}$ (3.34)

be any odd polynomial with real coefficients. By the definitions of the polynomial operation and the power operation, we have

$$\hat{\psi}\{M_N\} = c_1\{M_N\}^1 + c_3\{M_N\}^3 + \ldots + c_{2n+1}\{M_N\}^{2n+1}.$$
(3.35)

However, by theorem 4 and the relation

$$\{M_N\}^k = \{M_N\}^{k-1} \circ \{M_N\}$$
(3.36)

valid for $k \in \mathbb{Z}^+$, it follows that

$$\{M_N\}^{2m+1} \in X_d^-(q_1, q_2)$$
 (3.37)

for m = 0, 1, 2, ..., n. Since $X_d^-(q_1, q_2)$ is a linear space, by (3.35) and (3.37) one obtains

$$\hat{\psi}\{M_N\} \in X_d^-(q_1, q_2), \tag{3.38}$$

from which we are led to the conclusion.

It is well known that adjacency matrix A of any alternant can be written in the partitioned form,

$$A = \left(\frac{\text{zeros} \mid B}{B^{\text{T}} \mid \text{zeros}}\right),\tag{3.39}$$

where B is a $q_1 \times q_2$ real matrix with $q_1, q_2 \in \mathbb{Z}^+$ [15-17]. Thus, $\{M_N\} \in X_d(q)$, $q = q_1 + q_2$, defined by

$$M_N = B - \operatorname{diag}(\underbrace{A, A, \ldots, A}_{N})$$
(3.40)

is an element of $X_d^-(q_1, q_2)$.

We wish to have the following

THEOREM 6

Let $\{M_N\} \in X_d^-(q_1, q_2)$ be a fixed minus diagonal sequence with block-size (q_1, q_2) . Let I = [-a, a] be a closed interval compatible with $\{M_N\}$. Let α be the alpha functional of $\{M_N\}$ with domain C(I). Then the following equalities are true:

(i)
$$\alpha(P_0) = \{0\},$$
 (3.41)

(ii)
$$\alpha(C_0) = \{0\},$$
 (3.42)

where P_0 and C_0 are defined as in proposition 2.

Proof

(i) By theorem 5 and the definition of $X_d(q_1, q_2)$, for any $\varphi \in P_0$, all the diagonal elements of matrices $\varphi(M_N)$ vanish so that $\alpha(\varphi) = 0$.

(ii) By (i) and proposition 2, the conclusion follows.

COROLLARY

Let $q_1, q_2 \in \mathbb{Z}^+$, and let $\{M_N\} \in X_d^-(q_1, q_2)$. Then the spectrum of M_1 (which is contained in the real line) is symmetric around the origin; moreover, the algebraic multiplicities of the pairing eigenvalues coincide.

Proof

For each $\chi \in (0, a]$ and small enough $\varepsilon > 0$, consider a function $\varphi_{\chi,\varepsilon} \in C_0(I)$ such that $\varphi_{\chi,\varepsilon}(\pm \chi) = \pm 1$ and that the values of $\varphi_{\chi,\varepsilon}$ vanish except on the ε -neighbourhoods of χ and $-\chi$.

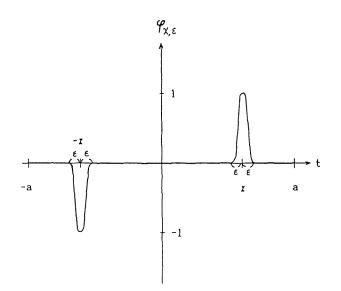


Fig. 1. A sketch of the function $\varphi_{\gamma,\epsilon}$.

Then theorem 6(ii) implies that

$$\alpha(\varphi_{\chi,\varepsilon}) = \sum_{i=1}^{q} \varphi_{\chi,\varepsilon}(\lambda_i(M_1)) = 0, \qquad (3.43)$$

from which the conclusion follows immediately.

Now we can immediately derive the spectral symmetry of alternants, or the spectral symmetry of the adjacency matrix A given in (3.39), using the above corollary (put $M_1 = A$), which has been obtained in parallel with the Alpha Space Asymptotic Linearity Theorem through the approach via the aspects of form and general topology.

4. Concluding remarks

We remark that all the theorems (i) αET , (ii) αIT , (iii) αRT , (iv) ALT, which are listed in the beginning of section 2, can be proved in two steps:

262

(I)
$$\pi(S) = \{T\},$$
 (4.1)

(II)
$$\pi(S) = \{T\},$$
 (4.2)

where π denotes a continuous mapping from a normed space E_1 to a non-Hausdorff topological space E_2 , and S denotes a subset of E_1 ; $\{T\}$ denotes a closed singleton set in E_2 (see ref. [5] for details).

These theorems (i)-(iv) can also be derived in two steps similar to those used in the present paper.

We shall here give a sketch only for the α Existence Theorem. Define a continuous functional $\omega_{\alpha}: C(I) \to \mathbb{R}$ by

$$\omega_{\alpha} = g \circ f_{\alpha} , \qquad (4.3)$$

where two continuous mappings $f_{\alpha}: C(I) \to \mathbb{R}^2$ and $g: \mathbb{R}^2 \to \mathbb{R}$ are defined by

$$f_{\alpha}(\varphi) = (\overline{\alpha}(\varphi), \underline{\alpha}(\varphi)), \tag{4.4}$$

$$g(x_1, x_2) = x_1 - x_2, \tag{4.5}$$

and where $\overline{\alpha}$, $\underline{\alpha}$ are defined by (3.7) and (3.8), respectively (cf. ref. [5] for the continuity of f_{α}).

Then we can prove the α Existence Theorem in two steps:

(i)
$$\omega_{\alpha}(P) = \{0\},$$
 (4.6)

(ii)
$$\omega_{\alpha}(\overline{P}) = \{0\},$$
 (4.7)

as we proved the X_{α} ALT and theorem 6 in the present paper.

References

- [1] S. Arimoto, Phys. Lett. 113A(1985)126.
- [2] S. Arimoto, Phys. Lett. 124A(1987)131.
- [3] S. Arimoto, Phys. Lett. 124A(1987)275.
- [4] S. Arimoto and G.G. Hall, Int. J. Quant. Chem. 41(1992)613.
- [5] S. Arimoto and M. Spivakovsky, J. Math. Chem. 13(1993)217.
- [6] T.L. Cottrell, J. Chem. Soc. (1948) 1448.
- [7] K.S. Pitzer and E. Catalano, J. Am. Chem. Soc. 78(1956)4844.
- [8] H. Shingu and T. Fujimoto, J. Chem. Phys. 31(1959)556.
- [9] H. Shingu and T. Fujimoto, Bull. Japan Petroleum Inst. 1(1959)11.
- [10] T. Fujimoto and H. Shingu, Nippon Kagaku Zasshi 82(1961)789, 794, 945, 948.
- [11] T. Fujimoto and H. Shingu, Nippon Kagaku Zasshi 83(1962)19.
- [12] T. Fujimoto and H. Shingu, Nippon Kagaku Zasshi 83(1962)23, 359, 364.
- [13] J.M. Schulman and R.L. Disch, Chem. Phys. Lett. 133(1985)291.
- [14] M.C. Flanigan, A. Kormornicki and J.W. McIver, Jr., in: *Electronic Structure Calculation*, ed. G.A. Segel (Plenum Press, New York, 1977).

- [15] G.G. Hall, Proc. Roy. Soc. A229(1955)251.
- [16] G.G. Hall, Int. J. Math. Educ. Sci. Technol. 4(1973)233.
- [17] G.G. Hall, Bull. Inst. Math. Appl. 17(1981)70.
- [18] J. Aihara, J. Am. Chem. Soc. 98(1976)2750.
- [19] A. Graovac, I. Gutman and N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules (Springer, Berlin, 1977).
- [20] I. Gutman and N. Trinajstić, Chem. Phys. Lett. 20(1973)257.
- [21] A.T. Balaban, Chemical Applications of Graph Theory (Academic Press, New York, 1976).
- [22] A. Tang, Y. Kiang, G. Yan and S. Tai, Graph Theoretical Molecular Orbitals (Science Press, Beijing, 1986).
- [23] Y. Jiang, A. Tang and R. Hoffmann, Theor. Chim. Acta 66(1984)183.
- [24] A. Motoyama and H. Hosoya, J. Math. Phys. 18(1977)1485.
- [25] H. Hosoya and A. Motoyama, J. Math. Phys. 26(1985)157.
- [26] R.B. Mallion and D.H. Rouvray, J. Math. Chem. 5(1990)1.