Journal of Statistical Physics, Vol. 75, Nos. 3/4, 1994

On the Leading Term and the Degree of the Polynomial Trace Mapping Associated with a Substitution

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Received January 25, 1993; final September 14, 1993

Using the trace mapping and the reduced trace mapping associated with a substitution, one obtaines the spectral properties of one-dimensional Schrödinger operators of the form $H = -\Delta + V$ on $l^2(\mathbb{Z})$, where Δ is the discrete Laplacian and V is a diagonal operator with elements derived from a substitution rule. In particular, the reduced trace mapping is closely related to the leading term of the original trace mapping. In this paper, the explicit expression of the leading term is given and its properties are discussed.

KEY WORDS: Trace maping; substitution; leading term.

1. INTRODUCTION

Since the discovery of quasicrystals by Shechtman *et al.*[16] many authors have investigated nonperiodic ordered chains of atoms generated by a substitution rule[6] acting on a finite alphabet, with each letter representing either an atom or an interval between two neighboring atoms (see, in particular, refs. 7, 17, and 18 and references therein).

Various physical properties of such systems have been obtained in a dynamical map approach leading to a trace map[9-11,13] for a number of cases, including the Fibonacci chain, Thue–Morse,[2] period-doubling,[4] circle and ternary non-Pisot sequences[5]: spectral properties (scaling, critical effects, etc.), wave functions (localization and optic al properties),[3] lattice dynamical properties (phonons), transport properties (resistance),[8] and structure factor (x-ray diffraction).[12]

To determine explicitly the trace is difficult in the general case, since

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0022-4715/94/0500-0627$07.00/0

it involves the iteration of a polynomial mapping from $\mathbb{R}^3$ to $\mathbb{R}^3$ for substitution with two letters. The substitutions of two letters are particularly important, because of their special properties and the existence of a recursion formula of the trace of certain products of transfer matrices.[1] Recently an important tool was introduced by Bovier and Ghez,[5] who considered a reduced trace map in order to derive spectral properties of a one-dimensional Schrödinger operator

$$H = -\Delta + V \qquad \text{on} \quad l^2(\mathbb{Z})$$

where Δ is the discrete Laplacian and V is a diagonal operator whose elements V_n are obtained from a substitution rule. In the two-letter case the reduced map leads to the leading terms of the original trace map.

The derivation of such leading terms is precisely the aim of this note. The leading term of a polynomial can offer much important information on it (see, e.g., ref. 15).

The article is organized as follows: In Section 2 we recall some definitions and introduce the notions of width and negative subword of a reduced word $w \in F$. Section 3 is devoted to the calculation of the leading term of the polynomial $\operatorname{Tr} \phi(w)$ (the trace of the product of matrices associated with w). We find that the leading term is determined completely by the combinatorial properties of w (its width, its length, and the set of its negative subwords). In Section 4 we introduce the connection coefficient $\delta(w, u)$ of two words w and u and we study its properties. With these properties and the results of Section 3 we determine the leading term of the trace mapping defined by a substitution, and then give the recurrence formula for the degree of the nth iteration of the trace polynomial. As we shall see, the combinatorial properties of the substitution still play an essential role. Some consequences are given and some examples are studied.

2. PRELIMINARY: DEFINITIONS AND NOTATIONS

Let $\mathcal{A} = \{a, b\}$ be a two-letter alphabet, $\mathcal{A}^*$ be the semigroup generated by $\mathcal{A}$, and F be the free group generated by $\mathcal{A}$. An element of F is also called a word. A word w is said to be reduced if there is no cancellation of letters in w, and $|w|$ denotes the number of the letters of w.

Let $SL_2(\mathbb{C})$ be the unimodular group over $\mathbb{C}$. Let ϕ be a homomorphism from F to $SL_2(\mathbb{C})$. Evidently, the restriction of ϕ on $\mathcal{A}^*$ is a homomorphism of the monoid $\mathcal{A}^*$.

We write $x = \operatorname{Tr} \phi(a)$, $y = \operatorname{Tr} \phi(b)$, and $z = \operatorname{Tr} \phi(ab)$, where Tr stands for the trace; then $\operatorname{Tr} \phi(w)$ is a polynomial of x, y, and z with coefficients in $\mathbb{Z}$.[1]

Let $w = x_1 x_2 \cdots x_k \in F$ ($x_i \in \mathcal{A}$) be a redcuced word; if $x_1 x_2 \cdots x_k x_1$ is also reduced, then w is called cyclic reduced. For any $w \in F$, we know easily that there exists a cyclic reduced word u such that $w = v^{-1} uv$ for some $v \in F$. We call u a cyclic reduced component of w. It is clear that $\operatorname{Tr} \phi(w) = \operatorname{Tr} \phi(u)$, and consequently we only need to consider the cyclic reduced words. In the remainder of the paper, unless stated otherwise, all the words will be considered as cyclic reduced. In particular, if $w \in \mathcal{A}^*$, then w is always cyclic reduced.

A subword $x_i x_{i+1} \cdots x_j$ of $w = x_1 x_2 \cdots x_k$ is called a negative subword in w if the letters $x_i, x_{i+1}, \ldots, x_{j-1}, x_j \in \mathcal{A}^{-1}$, and $x_{i-1}, x_{j+1} \in \mathcal{A}$ (where $x_s = x_{k+s}$ by convention). Moreover, if $x_{i-1} \neq x_{j+1}$ (which implies $x_i \neq x_j$), then the negative subword is called even.

Let $\alpha(w)$, $\beta(w)$ denote, respectively, the number of $a^{\pm 1}$, $b^{\pm 1}$ appearing in w. If $w \in \mathcal{A}^*$, then evidently $|w| = \alpha(w) + \beta(w)$.

The number of negative subwords in w is denoted by $\nu(w)$; in particular, if every letter in w belongs to $\mathcal{A}^{-1}$, we define $\nu(w) = 0$.

We call $\varepsilon(w)$ the number of even negative subwords of w. The number of $a^{\pm 1} b^{\pm 1}$ in $x_1 x_2 \cdots x_k x_1$ is called the width of w and is denoted by $\gamma(w)$.

Example 2.1. Let $w = ba^{-2}b^{-1}a^2ba^{-2}bab^{-2}a^{-3}b^2ab^{-3}a^{-2}b^{-2}a^2b^{-1}$.

A cyclic reduced component of w is $b^{-1}a^2ba^{-2}bab^{-2}a^{-3}b^2ab^{-3}a^{-2}b^{-2}$, and $a^{-2}, b^{-2}a^{-3}$, $b^{-3}a^{-2}b^{-2}b^{-1}$ are the negative subwords in w, and $b^{-2}a^{-3}$ is even. Thus $\alpha(w) = 11$, $\beta(w) = 12$ (but $|w| = 29$), $\gamma(w) = 6$, $\nu(w) = 3$, $\varepsilon(w) = 1$.

Let $w = x_1 x_2 \cdots x_k \in \mathcal{A}^*$ ($x_i \in \mathcal{A}$); we call a letter x_i isolated if $x_{i-1} = x_{i+1} \neq x_i$. The number of isolated letters a (resp. b) in w is called $\iota(w)$ [resp. $\kappa(b)$]. For instance, if $w = abbabaaba$, then $\iota(w) = 1$, $\kappa(w) = 2$.

A substitution σ over $\mathcal{A}$ can be considered as a homomorphism of $\mathcal{A}^*$, and its substitutive matrix is defined by

$$M_\sigma := \begin{pmatrix} \alpha(\sigma(a)) & \alpha(\sigma(b)) \\ \beta(\sigma(a)) & \beta(\sigma(b)) \end{pmatrix}$$

It is readily checked that

$$(\alpha(\sigma^n(w)), \beta(\sigma^n(w)))' = M_{\sigma^n}(\alpha(w), \beta(w))' = (M_\sigma)^n (\alpha(w), \beta(w))' \quad (2.1)$$

w_{first} (resp. w_{last}) will denote the first (resp. last) letter of w.

If $p(x, y, z)$ is a polynomial of variables x, y, and z, its degree will be denoted by $\deg(p)$ and its leading term will be denoted by $L(p)$. Moreover, $\deg_t(p)$ will denote the degree of p with respect to the variable t.

Let $c \in F$; then, by recurrence, using the Cayley–Hamilton theorem, we have for $n \in \mathbb{Z}$,

$$\phi(c^n) = p^n(u) \cdot \phi(c) - p_{n-1}(u) \cdot \mathrm{I} \quad (2.2)$$

where $u = \mathrm{Tr}\,\phi(c)$, I is the identity matrix, and $p_n(u)$ is the Chebychev polynomial with

$$p_n(u) = up_{n-1}(u) - p_{n-2}(u), \quad p_1(u) \equiv 1, \quad p_0(u) \equiv 0, \quad p_{-n}(u) = -p_n(u) \tag{2.3}$$

and

$$\deg(p_n(u)) = (n-1)\deg(u) \tag{2.4}$$

Thus

$$\mathrm{Tr}\,\phi(c^n) = up_n(u) - 2p_{n-1}(u) \tag{2.5}$$

and

$$\deg(\mathrm{Tr}\,\phi(c^n)) = n\deg(u) \tag{2.6}$$

It follows that

$$\mathrm{L}(\mathrm{Tr}\,\phi(c^n)) = \mathrm{L}(u^n) \tag{2.7}$$

3. THE LEADING TERM OF THE POLYNOMIAL Tr$\Phi(w)$

In this section, we will prove the following result:

Theorem 3.1. Let $w \in F$. Then the leading term of $\mathrm{Tr}\,\phi(w)$ is a monomial and

$$\mathrm{L}(\mathrm{Tr}\,\phi(w)) = (-1)^{\varepsilon(w)} x^{\alpha(w)-\gamma(w)+\nu(w)} y^{\beta(w)-\gamma(w)+\nu(w)} z^{\gamma(w)-\nu(w)}$$

In particular,

$$\deg(\mathrm{Tr}\,\phi(w)) = \alpha(w) + \beta(w) - \gamma(w) + \nu(w)$$

To prove this, we need first the following result.

Proposition 3.2. If $w \in \mathcal{O}^*$, then

$$\mathrm{L}(\mathrm{Tr}\,\phi(w)) = x^{\alpha(w)-\gamma(w)} y^{\beta(w)-\gamma(w)} z^{\gamma(w)}$$

In particular,

$$\deg(\mathrm{Tr}\,\phi(w)) = |w| - \gamma(w)$$

Proof. We proceed by induction on $\gamma(w)$. When $\gamma(w) = 0$, then $w = a^n$ (or b^n). In this case, $\alpha(w) = n$, $\beta(w) = 0$ [resp. $\alpha(w) = 0$, $\beta(w) = n$], hence from (2.7) the assertion is true for $\gamma(w) = 0$.

If $\gamma(w)>0$, as for any u, v one has $\operatorname{Tr}\phi(uv)=\operatorname{Tr}\phi(vu)$, we may suppose that

$$w=a^{t_1}b^{t_2}\cdots a^{t_{2\gamma-1}}b^{t_{2\gamma}}, \qquad \text{where} \quad \gamma=\gamma(w), \quad t_i>0$$

Now we assume that this proposition is true for words w with $\gamma(w)\leqslant\gamma$ and we shall prove that the conclusion is true for $\gamma+1$. It is clear that

$$\gamma(wa^nb^m)=\gamma(w)+1, \quad \alpha(wa^nb^m)=\alpha(w)+n, \quad \beta(wa^nb^m)=\beta(w)+m \quad (3.1)$$

1. First we consider the case $n=m=1$. Let

$$w'=a^{t_1}b^{t_2}\cdots a^{t_{2\gamma-3}}b^{t_{2\gamma-2}}$$

Thus

$$\alpha(w)=\alpha(w')+t_{2\gamma-1}, \qquad \beta(w)=\beta(w')+t_{2\gamma}, \qquad \gamma(w)=\gamma(w')+1$$

From (2.2)

$$\begin{aligned}\phi(wab)&=\phi(w')(p_{t_{2\gamma-1}}(x)\,\phi(a)-p_{t_{2\gamma-1}-1}(x)\mathrm{I})\\&\quad\times(p_{t_{2\gamma}}(y)\,\phi(b)-p_{t_{2\gamma}-1}(y)\mathrm{I})\,\phi(ab)\\&=p_{t_{2\gamma-1}}(x)\,p_{t_{2\gamma}}(y)\,\phi(w')\,\phi((ab)^2)\\&\quad-p_{t_{2\gamma-1}}(x)\,p_{t_{2\gamma}-1}(y)\,\phi(w')\,\phi(a^2b)\\&\quad-p_{t_{2\gamma-1}-1}(x)\,p_{t_{2\gamma}}(y)\,\phi(w')\,\phi(bab)\\&\quad+p_{t_{2\gamma-1}-1}(x)\,p_{t_{2\gamma}-1}(y)\,\phi(w')\,\phi(ab)\end{aligned} \qquad (3.2)$$

By the induction hypothesis and from (2.4), (2.7), (3.1), and (3.2) we have

$$\begin{aligned}&\mathrm{L}(\operatorname{Tr}(p_{t_{2\gamma-1}}(x)\,p_{t_{2\gamma}-1}(y)\,\phi(w')\,\phi(a^2b)))\\&\quad=x^{(\alpha(w')+2)-\gamma+(t_{2\gamma-1}-1)}\,y^{(\beta(w')+1)-\gamma+(t_{2\gamma}-2)}\,z^{\gamma}\\&\quad=x^{\alpha(w)-\gamma+1}\,y^{\beta(w)-\gamma-1}\,z^{\gamma}\end{aligned} \qquad (3.3)$$

$$\begin{aligned}&\mathrm{L}(\operatorname{Tr}(p_{t_{2\gamma-1}-1}(x)\,p_{t_{2\gamma}}(y)\,\phi(w')\,\phi(bab)))\\&\quad=x^{(\alpha(w')+1)-\gamma+(t_{2\gamma-1}-2)}\,y^{(\beta(w')+2)-\gamma+(t_{2\gamma}-1)}\,z^{\gamma}\\&\quad=x^{\alpha(w)-\gamma-1}\,y^{\beta(w)-\gamma+1}\,z^{\gamma}\end{aligned} \qquad (3.4)$$

$$\begin{aligned}&\mathrm{L}(\operatorname{Tr}(p_{t_{2\gamma-1}-1}(x)\,p_{t_{2\gamma}-1}(y)\,\phi(w')\,\phi(ab)))\\&\quad=x^{(\alpha(w')+1)-\gamma+(t_{2\gamma-1}-2)}\,y^{(\beta(w')+1)-\gamma+(t_{2\gamma}-2)}\,z^{\gamma}\\&\quad=x^{\alpha(w)-\gamma-1}\,y^{\beta(w)-\gamma-1}\,z^{\gamma}\end{aligned} \qquad (3.5)$$

On the other hand,

$$\phi(w'(ab)^2) = \phi(w')(z\phi(ab) - \mathrm{I}) = z\phi(w'ab) - \phi(w')$$

Thus

$$\begin{aligned} &\mathrm{L}(\mathrm{Tr}(p_{t_{2\gamma-1}}(x)\, p_{t_{2\gamma}} \phi(y)(w')\, \phi((ab)^2))) \\ &\quad = x^{(\alpha(w')+1)-\gamma+(t_{2\gamma-1}-1)}\, y^{(\beta(w')+1)-\gamma+(t_{2\gamma}-1}\, z^{\gamma+1} \\ &\quad = x^{(\alpha(w)+1)-(\gamma+1)}\, y^{(\beta(w)+1)-(\gamma+1)}\, z^{\gamma+1} \end{aligned} \tag{3.6}$$

So that from the equalities above, we have

$$\mathrm{L}(\mathrm{Tr}\, \phi(wab)) = x^{(\alpha(w)+1)-(\gamma+1)}\, y^{(\beta(w)+1)-(\gamma+1)}\, z^{\gamma+1} \tag{3.7}$$

2. For the general case of m, n, by (2.2), we have

$$\begin{aligned} \phi(wa^n b^m) &= \phi(w)(p_n(x)\, \phi(a) - p_{n-1}(x)\mathrm{I})(p_m(y)\, \phi(b) - p_{m-1}(y)\mathrm{I}) \\ &= p_n(x)\, p_m(y)\, \phi(wab) - p_n(x)\, p_{m-1}(y)\, \phi(wa) \\ &\quad - p_{n-1}(x)\, p_m(y)\, \phi(wb) + p_{n-1}(x)\, p_{m-1}(y)\, \phi(w) \end{aligned} \tag{3.8}$$

By means of the hypothesis of induction and step 1, we obtain finally that

$$\mathrm{L}(\mathrm{Tr}\, \phi(wa^n b^m)) = x^{(\alpha(w)+n)-(\gamma+1)}\, y^{(\beta(w)+m)-(\gamma+1)}\, z^{\gamma+1} \tag{3.9}$$

We have thus proved this proposition by induction.

Proposition 3.3. Let $w \in \mathcal{A}^*$. We have

$$\deg_x(\mathrm{Tr}\, \phi(w)) = \alpha(w) - \kappa(w)$$

$$\deg_y(\mathrm{Tr}\, \phi(w)) = \beta(w) - \iota(w)$$

$$\deg_z(\mathrm{Tr}\, \phi(w)) = \gamma(w)$$

The proof of this proposition is similar to that of Proposition 3.2. Furthermore, we can also determine the respective leading term.

Proof of Theorem 3.1. We proceed by induction on $\nu(w) = \nu$. The case of $\nu(w) = 0$ is just Proposition 3.2. Assume that this theorem is true for $\nu(w) \leqslant \nu - 1$ and we consider the case of $\nu(w) = \nu \geqslant 1$. Hence, there exists at least a negative subword u in w, and, without changing the trace, w can be rewritten as uv, where v is not the empty word. Notice that

$$\alpha(u^{-1}) = \alpha(u), \qquad \beta(u^{-1}) = \beta(u), \qquad \gamma(u^{-1}) = \gamma(u) \tag{3.10}$$

$$\alpha(w) = \alpha(u^{-1}v) = \alpha(u) + \alpha(v) \tag{3.11}$$

$$\beta(w) = \beta(u^{-1}v) = \beta(u) + \beta(v) \tag{3.12}$$

$$\gamma(w) = \gamma(u^{-1}v) \tag{3.13}$$

$$\nu(v) = \nu(u^{-1}v) = \nu(w) - 1 \tag{3.14}$$

Now, from (2.2)

$$\phi(u) = \mathrm{Tr}\,\phi(u^{-1})\mathrm{I} - \phi(u^{-1})$$

so we have

$$\phi(w) = \phi(uv) = (\mathrm{Tr}\,\phi(u^{-1})\mathrm{I} - \phi(u^{-1}))\,\phi(v) = (\mathrm{Tr}\,\phi(u^{-1}))\,\phi(v) - \phi(u^{-1})\,\phi(v)$$

i.e.,

$$\mathrm{Tr}\,\phi(w) = (\mathrm{Tr}\,\phi(u^{-1}))(\mathrm{Tr}\,\phi(v)) - \mathrm{Tr}\,\phi(u^{-1}v) \tag{3.15}$$

1. If u is not even, then by the definition,

$$u^{-1}_{\text{first}} = u^{-1}_{\text{last}} \neq v_{\text{first}} = v_{\text{last}}$$

which implies that

$$\gamma(u^{-1}) + \gamma(v) = \gamma(u^{-1}v) - 1 = \gamma(w) - 1 \tag{3.16}$$

and

$$\varepsilon(v) = \varepsilon(u^{-1}v) = \varepsilon(w) \tag{3.17}$$

Thus, from (3.10)–(3.17) and Proposition 3.2,

$$\begin{aligned} &\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}))(\mathrm{Tr}\,\phi(v)) \\ &\quad = x^{\alpha(u)-\gamma(u)}\, y^{\beta(u)-\gamma(u)}\, z^{\gamma(u)} (-1)^{\varepsilon(v)} x^{\alpha(v)-\gamma(v)+\nu(v)}\, y^{\beta(v)-\gamma(v)+\nu(v)}\, z^{\gamma(v)-\nu(v)} \\ &\quad = (-1)^{\varepsilon(w)} x^{\alpha(w)-\gamma(w)+\nu(w)}\, y^{\beta(w)-\gamma(w)+\nu(w)}\, z^{\gamma(w)-\nu(w)} \end{aligned}$$

On the other hand,

$$\begin{aligned} &\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}v)) \\ &\quad = (-1)^{\varepsilon(u^{-1}v)} x^{\alpha(u^{-1}v)-\gamma(u^{-1}v)+\nu(u^{-1}v)}\, y^{\beta(u^{-1}v)-\gamma(u^{-1}v)+\nu(u^{-1}v)}\, z^{\gamma(u^{-1}v)-\nu(u^{-1}v)} \\ &\quad = (-1)^{\varepsilon(w)} x^{\alpha(w)-\gamma(w)+\nu(w)-1}\, y^{\beta(w)-\gamma(w)+\nu(w)-1}\, z^{\gamma(w)-\nu(w)+1} \end{aligned}$$

By comparing the two formulas above, we obtain

$$\deg(\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1})\,\mathrm{Tr}\,\phi(v))) > \deg(\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}v)))$$

Therefore

$$\begin{aligned}\mathrm{L}(\mathrm{Tr}\,\phi(w)) &= \mathrm{L}(\mathrm{Tr}\,\phi(u^{-1})\,\mathrm{Tr}\,\phi(v))\\ &= (-1)^{\varepsilon(w)} x^{\alpha(w)-\gamma(w)+\nu(w)} y^{\beta(w)-\gamma(w)+\nu(w)} z^{\gamma(w)-\nu(w)}\end{aligned}$$

2. If u is even, then

$$u^{-1}_{\text{first}} = v_{\text{last}} \neq u^{-1}_{\text{last}} = v_{\text{first}}$$

so that

$$\gamma(u^{-1}) + \gamma(v) = \gamma(u^{-1}v) + 1 = \gamma(w) \tag{3.18}$$

and

$$\varepsilon(v) = \varepsilon(u^{-1}v) = \varepsilon(w) - 1 \tag{3.19}$$

In the same way as in step 1, and from (3.18) and (3.19), one has

$$\begin{aligned}&\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}))(\mathrm{Tr}\,\phi(v))\\ &\quad= x^{\alpha(u)-\gamma(u)} y^{\beta(u)-\gamma(u)} z^{\gamma(u)}(-1)^{\varepsilon(v)} x^{\alpha(v)-\gamma(v)+\nu(v)} y^{\beta(v)-\gamma(v)+\nu(v)} z^{\gamma(v)-\nu(v)}\\ &\quad= (-1)^{\varepsilon(w)-1} x^{\alpha(w)-\gamma(w)+\nu(w)-1} y^{\beta(w)-\gamma(w)+\nu(w)-1} z^{\gamma(w)-\nu(w)+1}\\ &\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}v))\\ &\quad= (-1)^{\varepsilon(u^{-1}v)} x^{\alpha(u^{-1}v)-\gamma(u^{-1}v)+\nu(u^{-1}v)} y^{\beta(u^{-1}v)-\gamma(u^{-1}v)+\nu(u^{-1}v)} z^{\gamma(u^{-1}v)-\nu(u^{-1}v)}\\ &\quad= (-1)^{\varepsilon(w)-1} x^{\alpha(w)-\gamma(w)+\nu(w)} y^{\beta(w)-\gamma(w)+\nu(w)} z^{\gamma(w)-\nu(w)}\end{aligned}$$

and

$$\deg(\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1})\,\mathrm{Tr}\,\phi(v))) < \deg(\mathrm{L}(\mathrm{Tr}\,\phi(u^{-1}v)))$$

We obtain also that

$$\begin{aligned}\mathrm{L}(\mathrm{Tr}\,\phi(w)) &= \mathrm{L}(-(\mathrm{Tr}\,\phi(u^{-1}v)))\\ &= (-1)^{\varepsilon(w)} x^{\alpha(w)-\gamma(w)+\nu(w)} y^{\beta(w)-\gamma(w)+\nu(w)} z^{\gamma(w)-\nu(w)}\end{aligned}$$

Thus using steps 1 and 2, one finishes the reasoning by induction.

Evidently, decreasing a $a^{\pm 1}b^{\pm 1}$ in w means decreasing at least a $a^{\pm 1}$ (or $b^{\pm 1}$). Let u be a subword of w; it is easy to see that $\gamma(w) - \gamma(w) \leqslant$

$|w| - |u|$, i.e., $|w| - \gamma(w) \geqslant |u| - \gamma(u)$. On the other hand, it is clear that $v(w) \geqslant v(u)$. So by Theorem 3.1, we have the inequality

$$\deg(\mathrm{Tr}\,\phi(w)) \geqslant \deg(\mathrm{Tr}\,\phi(u))$$

We have the following result.

Corollary 3.4. The degree of the polynomial $\mathrm{Tr}\,\phi(w)$ is not decreased by eliminating any subword of w.

Furthermore, we have the following corollaries.

Corollary 3.5. Let $w \in F$. If w is not the empty word, then $\deg(\mathrm{Tr}\,\phi(w)) > 0$.

Corollary 3.6. Let $w \in F$. If $\gamma(w) \geqslant 2$ and $w \neq (a^{\pm 1}b^{\pm 1})^m$, then $\mathrm{L}(\mathrm{Tr}\,\phi(w))$ is divisible by xyz

Remark. Let $x^\alpha y^\beta z^\gamma$ be a monomial of variables x, y, and z; then its weight is defined by $\alpha + \beta + 2\gamma$. The weight of a polynomial $p(x, y, z)$, which is called $\omega(p)$, is the maximum of the weights of all its monomials. By induction, we can prove the following:

Proposition 3.7. Let $w \in F$; then

$$\omega(\mathrm{Tr}\,\phi(w)) = \omega(\mathrm{L}(\mathrm{Tr}\,\phi(w))) = \alpha(w) + \beta(w)$$

In particular, if $w \in \mathcal{C}^*$, then

$$\omega(\mathrm{Tr}\,\phi(w)) = \omega(\mathrm{L}(\mathrm{Tr}\,\phi(w))) = |w|$$

We see that the polynomial $\mathrm{Tr}\,\phi(w)$ may take its weight by its leading term.

But in general, the leading term is not the unique term with the above property; for example, we have

$$\mathrm{Tr}\,\phi(a^{-1}b^{-1}ab) = x^2 + y^2 + z^2 - xyz - 2$$

with

$$\omega(z^2) = \omega(xyz) = \omega(\mathrm{Tr}\,\phi(a^{-1}b^{-1}ab)) = 4$$

4. THE LEADING TERM AND THE DEGREE OF THE TRACE MAPPING POLYNOMIAL

Throughout this section, we confine ourselves to $\mathcal{C}^*$. In this case, any word of $\mathcal{C}^*$ is cyclic reduced and it has no negative subword.

Let $u, v \in \mathcal{A}^*$; we are going to determine the leading term of Tr $\phi(uv)$. In order to study the relation between the width of uv and that of u and v, we define the connection coefficient of u, v, denoted by $\delta(u, v)$, as follows:

$$\delta(u, v) = \gamma(u) + \gamma(v) - \gamma(uv)$$

Then by Proposition 3.2,

$$\mathrm{L}(\mathrm{Tr}\, \phi(uv)) = \mathrm{L}(\mathrm{Tr}\, \phi(u)) \cdot \mathrm{L}(\mathrm{Tr}\, \phi(v)) \cdot (xyz^{-1})^{\delta(u,v)}$$

and we see that L(Tr $\phi(uv)$) will be determined by $\delta(u, v)$. Thus, we first study the properties of the connection coefficients. The following result is readily checked.

Lemma 4.1. Let $u, v \in \mathcal{A}^*$. We have

$$\delta(u, v) = \begin{cases} 1 & \text{if} \quad u_{\text{first}} = u_{\text{last}} \neq v_{\text{first}} = v_{\text{last}} \\ -1 & \text{if} \quad u_{\text{first}} = v_{\text{last}} \neq v_{\text{first}} = u_{\text{last}} \\ 0 & \text{otherwise} \end{cases}$$

By Theorem 3.1 and the definition of δ, we obtain immediately the following result:

Corollary 4.2. For $w, u \in \mathcal{A}^*$, we have:

(i) $\mathrm{L}(\mathrm{Tr}\, \phi(wu)) = \mathrm{L}(\mathrm{Tr}\, \phi(w))\, \mathrm{L}(\mathrm{Tr}\, \phi(u))\, z^{\delta(w,u)}$.

(ii) $\deg(\mathrm{Tr}\, \phi(wu)) = \deg(\mathrm{Tr}\, \phi(w)) + \deg(\mathrm{Tr}\, \phi(u)) + \delta(w, u)$.

(iii) If u is a subword of w, then

$$\mathrm{L}(\mathrm{Tr}\, \phi(u)) \mid \mathrm{L}(\mathrm{Tr}\, \phi(w))$$

It is convenient to give below some simple formulas which are consequences of Lemma 4.1.

Proposition 4.3. For $w, u \in \mathcal{A}^*$, we have the following assertions:

(i) $\delta(w, u) = \delta(u, w)$.

(ii) $\delta(w, w) = 0$.

(iii) $\delta(w^m, u^n) = \delta(w, u)$, $m, n \in \mathbb{N} \setminus \{0\}$.

(iv) $\gamma(wu) = \gamma(wu)$.

(v) $\gamma(w^m) = m\gamma(w)$, $m \in \mathbb{N}$.

(vi) $\gamma(w^m u^n) = m\gamma(w) + n\gamma(u) - \delta(w, u)$, $m, n \in \mathbb{N} \setminus \{0\}$.

(vii) If $w = u^{t_1} v^{t_2} \cdots u^{t_{2\gamma-1}} v^{t_{2\gamma}}$, then

$$\gamma(w) = (t_1 + t_3 + \cdots + t_{2\gamma-1})\, \gamma(u) + (t_2 + t_4 + \cdots + t_{2\gamma})\, \gamma(v) + \gamma\delta(u, v)$$

Proof. Assertions (i), (ii) follow immediatly from Lemma 4.1.

We have $w^m_{\text{first}} = w_{\text{first}}$, $w^m_{\text{last}} = w_{\text{last}}$ for $m \in \mathbb{Z}\backslash\{0\}$, hence (iii). Assertion (iv) comes from the definition of δ and (i). Assertion (v) comes from the definition of δ and (ii). By the definition of δ again, and from (iii), (v), we have

$$\gamma(w^m u^n) = \gamma(w^m) + \gamma(u^n) - \delta(w^m, u^n) = m\gamma(w^m) + n\gamma(u^m) - \delta(w, u)$$

which implies (vi). Finally, (vii) follows from (vi) by induction.

Let σ be a substitution over $\mathcal{A}$. Define

$$\delta(\sigma) = \delta(\sigma(a), \sigma(b))$$

Proposition 2.4. Let σ be a substitution over $\mathcal{A}$. We have that for $u, v, w \in \mathcal{A}^*$:

(i) $\delta(\sigma(u), \sigma(v)) = \delta(\sigma)\, \delta(u, v)$.

(ii) $\delta(\sigma^n) = (\delta(\sigma))^n =: \delta^n(\sigma)$.

(iii) $\gamma(\sigma(w)) = \alpha(w)\, \gamma(\sigma(a)) + \beta(w)\, \gamma(\sigma(b)) + \gamma(w)\, \delta(\sigma)$.

Proof. Part (i) follows from Lemma 4.1 by considering all possible cases of the first and last letters of the words u, v, $\sigma(a)$, $\sigma(b)$.

Part (ii) follows from (i) by induction. Part (iii) follows from Proposition 4.3(iv), (vii).

Theorem 4.5. Let σ be a substitution over $\mathcal{A}$. Then

$$\gamma(\sigma^{n+1}) = \gamma(\sigma)(\mathrm{M}^n + \delta\mathrm{M}^n + \cdots + \delta^{n-1}\mathrm{M} + \delta^n\mathrm{I}) \tag{4.1}$$

where $\mathrm{M} := \mathrm{M}_\sigma$, $\delta := \delta(\sigma)$, $\gamma(\sigma^n) := (\gamma(\sigma^n(a)), \gamma(\sigma^n(b)))$, $n \in \mathbb{N}$.

In particular, if the matrix $\mathrm{M} - \delta\mathrm{I}$ is invertible, then

$$\gamma(\sigma^n) = \gamma(\sigma)(\mathrm{M} - \delta\mathrm{I})^{-1}(\mathrm{M}^n - \delta^n\mathrm{I}) \tag{4.1'}$$

Proof. We proceed by induction. This is trival when $n = 0$.

Assume by induction that (4.1) is true for n. From Proposition 4.4(iii),

$$\begin{aligned}\gamma(\sigma^{n+1}(a)) &= \gamma(\sigma(\sigma^n(a)))\\ &= \alpha(\sigma^n(a))\, \gamma(\sigma(a)) + \beta(\sigma^n(a))\, \gamma(\sigma(b)) + \gamma(\sigma^n(a))\, \delta(\sigma)\end{aligned}$$

By the hypothesis of induction and the equality (2.1) we have

$$\begin{aligned}\gamma(\sigma^{n+1}(a)) &= \alpha(\sigma^n(a))\, \gamma(\sigma(a)) + \beta(\sigma^n(a))\, \gamma(\sigma(b)) + \gamma(\sigma^n(a))\, \delta(\sigma)\\ &= \gamma(\sigma)\, \mathrm{M}^n(1, 0)' + \gamma(\sigma)(\mathrm{M}^{n-1} + \delta\mathrm{M}^{n-2} + \cdots\\ &\quad + \delta^{n-2}\mathrm{M} + \delta^{n-1}\mathrm{I})\, \delta(\sigma)(1, 0)'\\ &= \gamma(\sigma)(\mathrm{M}^n + \delta\mathrm{M}^n + \cdots + \delta^{n-1}\mathrm{M} + \delta^n\mathrm{I})(1, 0)' \end{aligned} \tag{4.2}$$

In the same way,

$$\gamma(\sigma^{n+1}(b)) = \gamma(\sigma)(\mathrm{M}^n + \delta\mathrm{M}^n + \cdots + \delta^{n-1}\mathrm{M} + \delta^n\mathrm{I})(0, 1)' \qquad (4.3)$$

Thus (4.1) follows from (4.2) and (4.3) and the assertion is true for every $n \in \mathbb{N}$.

Keep the notations of Section 3. Let $\phi \in \mathrm{Hom}(F, SL_2(\mathbb{C}))$ as above; then ϕ is uniquely determined by the couple $(\phi(a), \phi(b))$ of elements of $SL_2(\mathbb{C})$. Now define a mapping T: $\mathrm{Hom}(F, SL_2(\mathbb{C})) \to \mathbb{C}^3$, $T(\phi) = (\mathrm{Tr}\,\phi(a), \mathrm{Tr}\,\phi(b), \mathrm{Tr}\,\phi(ab))$. By ref. 1, for any $\sigma \in \mathrm{End}(F)$, there is a unique $\Phi_\sigma \in (\mathbb{Z}[x, y, z])^3$ such that

$$T(\phi \circ \sigma) = \Phi_\sigma(T(\phi))$$

The polynomial mapping Φ_σ is called the trace mapping associated with σ.

The following theorem is a direct corollary of Proposition 3.2, Proposition 4.4, and Theorem 4.5.

Theorem 4.6. Let σ be a substitution over $\mathcal{A}$ with the trace mapping Φ_σ, and let

$$\Phi_{\sigma^n} = (\Phi_{na}, \Phi_{nb}, \Phi_{nab})$$

be the nth iteration of Φ_σ. Let $x = \mathrm{Tr}\,\phi(a)$, $y = \mathrm{Tr}\,\phi(b)$, $z = \mathrm{Tr}\,\phi(ab)$; then

$$\mathrm{L}(\Phi_{nc}) = x^{e(n,c,x)}\, y^{e(n,c,y)}\, z^{e(n,c,z)}$$

where $c \in \{a, b, ab\}$ and $e(n, c, t)$ are determined by the following formulas ($t \in \{x, y, z\}$):

$$\begin{pmatrix} e(n, a, x) & e(n, b, x) \\ e(n, a, y) & e(n, b, y) \end{pmatrix} = \mathrm{M}_\sigma^n - \begin{pmatrix} 1 \\ 1 \end{pmatrix} \gamma(\sigma^n)$$

$$(e(n, a, z), e(n, b, z)) = \gamma(\sigma^n)$$

$$(e(n, ab, x), e(n, ab, y))' = ((\mathrm{M}_\sigma)^n - e(n, ab, z)\mathrm{I})(1, 1)'$$

$$e(n, ab, z) = \gamma(\sigma^n)(1, 1)' - \delta^n(\sigma)$$

Example 4.1. Fibonacci substitution: $\sigma(a) = ab$, $\sigma(b) = a$. Let $\{f(n)\}_{n \geq 0}$ be the Fibonacci sequence, that is, $f(-1) = 0$, $f(0) = 1$, $f(n) = f(n-1) + f(n-2)$ $(n \geq 1)$. It is well known that $|\sigma^n(a)| = f(n)$, $|\sigma^n(b)| = f(n-1)$; since $\sigma(a) = \sigma^2(b)$, we have $\alpha(\sigma^n(a)) = f(n-1)$ and $\alpha(\sigma^n(b)) = f(n-2)$.

Notice that $\gamma(\sigma)=(1,0)$, $\delta(\sigma(a),\sigma(b))=0$; then from Theorem 4.5

$$\gamma(\sigma^n)=(1,0)(\mathrm{M}_\sigma)^{n-1}=(|\sigma^{n-1}(a)|,|\sigma^{n-1}(b)|)=(f(n-1),f(n-2))$$

Hence

$$\mathrm{L}(\Phi_{na})=x^{f(n)-f(n-1)}y^{f(n-1)-f(n-1)}z^{f(n-1)}=x^{f(n-2)}z^{f(n-1)}$$
$$\mathrm{L}(\Phi_{nb})=x^{f(n-3)}z^{f(-2)}(x^{f(-2)}=y \text{ by convention})$$
$$\mathrm{L}(\Phi_{nab})=x^{f(n-1)}z^{f(n)}$$

In particular,

$$\deg(\mathrm{Tr}\,\phi(\sigma^n(a)))=f(n), \qquad \deg(\mathrm{Tr}\,\phi(\sigma^n(b)))=f(n-1)$$
$$\deg(\mathrm{Tr}\,\phi(\sigma^n(ab)))=f(n+1)$$

are still the terms of the Fibonacci sequence; thus the sequence $\{\deg \mathrm{Tr}\,\phi(\sigma^n(a))\}_{n\geq 0}$ is still the Fibonacci sequence.

Example 4.2. (See also ref. 2.) Thue–Morse substitution: $\sigma(a)=ab$, $\sigma(b)=ba$. We have then $\gamma(\sigma)=(1,1)$, $\delta(\sigma(a),\sigma(b))=-1$. In this case, $\mathrm{M}_\sigma^n=2^n\mathrm{M}_\sigma$, and

$$\mathrm{M}_\sigma-\delta\mathrm{I}=\begin{pmatrix}2 & 1\\ 1 & 2\end{pmatrix}$$

is invertible, so by (4.1′)

$$\gamma(\sigma^n)=(1,1)\begin{pmatrix}2 & 1\\ 1 & 2\end{pmatrix}^{-1}\left(2^{n-1}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}-(-1)^n\mathrm{I}\right)$$
$$=\left(\frac{2^n-(-1)^n}{3},\frac{2^n-(-1)^n}{3}\right)$$

Thus, by Theorem 4.6,

$$e(n,a,x)=e(n,a,y)=e(n,b,x)=e(n,b,y)=e(n-1,a,z)$$
$$=e(n-1,b,z)=e(n-1,ab,x)=e(n-1,ab,y)$$
$$=(2^{n-1}-(-1)^{n-1})/3$$
$$e(n,ab,z)=(2^{n+1}-(-1)^{n+1})/3=\deg(\mathrm{L}\Phi_{na})$$
$$=\deg(\mathrm{L}\Phi_{nb})=\deg(\mathrm{L}\Phi_{(n-1)ab})$$

More generally, for the substitution $\sigma(a)=a^pb^q$, $\sigma(b)=b^qa^p$, $\gamma(\sigma)=(1,1)$, $\delta(\sigma)=-1$,

$$\mathrm{M}_\sigma=\begin{pmatrix} p & p \\ q & q \end{pmatrix}, \qquad \mathrm{M}_\sigma-\delta\mathrm{I}=\begin{pmatrix} p+1 & p \\ q & q+1 \end{pmatrix}$$

$$\mathrm{M}_\sigma^n=\frac{1}{2}\begin{pmatrix} (p+q)^n+(p-q)^n & (p+q)^n-(p-q)^n \\ (p+q)^n-(p-q)^n & (p+q)^n+(p-q)^n \end{pmatrix}$$

$$\gamma(\sigma^n)=(1,1)\begin{pmatrix} p+1 & p \\ q & q+1 \end{pmatrix}^{-1}(\mathrm{M}_\sigma^n-(-1)^n\mathrm{I})$$

$$=\left(\frac{(p+q)^n-(-1)^n}{p+q+1}, \frac{(p+q)^n-(-1)^n}{p+q+1}\right)$$

$$\deg\Phi_{na}=(p+q)^n-\frac{(p+q)^n-(-1)^n}{p+q+1}=\deg\Phi_{nb}$$

Let σ be a substitution over $\mathcal{A}$, Φ_σ be the corresponding trace mapping polynomial, and $\lambda=x^2+y^2+z^2-xyz-4$. To characterize the invariant domain by Φ_σ, Peyrière has shown the following facts[14]:

(i) There exists a polynomial $Q_\sigma\in\mathbb{Z}[x,y,z]$, such that

$$\lambda\circ\Phi_\sigma=\lambda\cdot Q_\sigma \tag{4.4}$$

(ii) If σ is invertible, then $Q_\sigma=1$.

Now we will determine the degree of Q_σ by $\delta(\sigma)$. From Theorem 4.6 and (4.4), a careful calculation, of which we omit the details, gives the following result.

Theorem 4.7. Let σ be a substitution over $\mathcal{A}$. We have:

(i) If $\delta(\sigma)=-1$, then $\deg(Q_\sigma)=2\deg(\Phi_{ab})-3>0$.

(ii) If $\delta(\sigma)=1$, then

$$\deg(Q_\sigma)=\deg(\Phi_a)+\deg(\Phi_b)+\deg(\Phi_{ab})-3>0.$$

(iii) If $\delta(\sigma)=0$, then

$$\deg(Q_\sigma)<2\deg(\Phi_{ab})-3=\deg(\Phi_a)+\deg(\Phi_b)+\deg(\Phi_{ab})-3.$$

Corollary 4.8. If σ is invertible, then $\delta(\sigma(a),\sigma(b))=0$.

In this case, $Q_\sigma=1$ implies that $\deg(Q_\sigma)=0$, and the result comes by Theorem 4.7.

ACKNOWLEDGMENTS

The authors thank Prof. J. Peyrière for useful discussions and Prof. A. Janner for his kind help. Z.-Y.W. is grateful to CNRS for financial support and to the Laboratory of Solid Physics at Orsay for hospitality.

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