Positive Eigenvalues of Generalized Words in Two Hermitian Positive Definite Matrices*

Christopher J. Hillar† and Charles R. Johnson‡

Abstract. We define a word in two positive definite (complex Hermitian) matrices A and B as a finite product of real powers of A and B. The question of which words have only positive eigenvalues is addressed. This question was raised some time ago in connection with a long-standing problem in theoretical physics, and it was previously approached by the authors for words in two real positive definite matrices with positive integral exponents. A large class of words that do guarantee positive eigenvalues is identified, and considerable evidence is given for the conjecture that no other words do.

Key words. positive definite matrix, generalized word, eigenvalues, nearly symmetric

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1. Introduction.

A *generalized word* (*g-word*, for short) $W = W(A, B)$ in two letters A and B is an expression of the form

$$W = A^{p_1} B^{q_1} A^{p_2} B^{q_2} \cdots A^{p_k} B^{q_k} A^{p_{k+1}}$$

in which the exponents p_i and q_i are real numbers such that $p_i, q_i \neq 0$, $i = 1, \ldots, k$, and p_{k+1} is an arbitrary real number. We call k the *class number* of W. The *reversal* of the g-word W is $W^* = A^{p_{k+1}} B^{q_k} A^{p_k} \cdots B^{q_2} A^{p_2} B^{q_1} A^{p_1}$ and a g-word is *symmetric* if it is identical to its reversal (in other contexts, the name "palindromic" is also used).

We are interested in the matrices that result when the two letters are (independent) positive definite (complex Hermitian) n-by-n matrices (PD, for short). For convenience, the letters A, B will also represent the substituted PD matrices (the context will make the distinction clear). To make sure that W is well-defined after substitution, we take primary PD powers (see [4, p.433] and [4, p.413]). I.e., given $p \in \mathbb{R}$, a unitary matrix U, and a positive diagonal matrix D, we have $(UDU^*)^p = UD^pU^*$.

We are primarily interested in those g-words for which W has only positive (real) eigenvalues, no matter what the positive definite matrices A and B are (for any positive integer n). We call such a g-word *good* and all other g-words *bad*. Interest in this problem stems from a question in quantum physics [1,7], as discussed in [5] for the case of (ordinary) words (p_i, q_i positive integers) and real symmetric positive definite matrices. For 2-by-2 matrices, the situation is better understood. For example, if all of the p_i or q_i are of the same sign, then it is known [2] that any word in two 2-by-2 PD matrices necessarily has positive eigenvalues. Since we are interested in those words that are bad, our search should begin with $n = 3$.

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† Department of Mathematics, University of California, Berkeley, CA 94720. (chillar@math.berkeley.edu). The work of the first author is supported under a National Science Foundation Graduate Research Fellowship

‡ Department of Mathematics, College of William and Mary, Williamsburg, VA 23187-8795. (crjohnso@math.wm.edu)

We call a g-word *nearly symmetric* if it is either symmetric or a product (juxtaposition) of two symmetric words. It is an elementary exercise that good g-words (and, therefore, bad also) are unchanged by each of the following:

i) reversal;
ii) interchange of the letters A,B;
iii) cyclic permutation, e.g.,

$$A^{p_1}B^{q_1}A^{p_2}B^{q_2}\cdots A^{p_k}B^{q_k} \longrightarrow B^{q_1}A^{p_2}B^{q_2}\cdots A^{p_k}B^{q_k}A^{p_1}.$$

iv) multiplication of all the p_i's (q_i's) by a fixed nonzero scalar.

It is also an elementary combinatorial exercise that each of (i)-(iv) preserves the nearly symmetric g-words.

Recall that two n-by-n matrices X and Y are said to be *congruent* if there is an invertible n-by-n matrix Z such that $Y = Z^*XZ$ and that congruence on Hermitian matrices preserves inertia (the ordered triple consisting of the number of positive, negative, and zero eigenvalues) and, thus, positive definiteness [3, p.223]. A symmetric word of class k in two positive definite matrices is congruent to one of class $k-1$, iteration of which implies congruence to the "center," class 0, positive definite matrix. We conclude that

Lemma 1.1. A symmetric g-word in two positive definite matrices is positive definite; thus, every symmetric g-word is good.

It is also known [3, p.465] that a product of two positive definite matrices has only positive eigenvalues. In view of Lemma 1.1, it then follows that

Theorem 1.2. Each nearly symmetric g-word is good.

We conjecture the converse to Theorem 1.2.

Conjecture 1.3. A g-word is good if and only if it is nearly symmetric.

We note that near symmetry is easily verified algorithmically. Using iii), each g-word W may be taken to be in the form in which $p_{k+1} = 0$, i.e. the g-word may be taken to begin with a power of one letter and end with a power of the other. We refer to this as *standard form.* Then, near symmetry of $A^{p_1}B^{q_1}A^{p_2}B^{q_2}\cdots A^{p_k}B^{q_k}$ may be determined by inspection of each pair of words of the form $A^{p_1}B^{q_1}A^{p_2}B^{q_2}\cdots A^{p_i}$, $B^{q_i}A^{p_{i+1}}B^{q_{i+1}}\cdots A^{p_k}B^{q_k}$, $i = 1,\ldots,k$.

The number of class k words that are nearly symmetric is small compared to the total number of all such words. Therefore, if Conjecture 1.3 were to be true, it is necessary that the "density" of good words is also 0. To make this precise, we view the space of good words (of class k) as a subset of $\mathbb{R}^{2k}$ parameterized by $\{(p_1, q_1, ..., p_k, q_k) \mid W \text{ is good}\}$. Our main theorem in this direction is then given by the following.

Theorem 1.3. The set of good words of class k has measure zero in $\mathbb{R}^{2k}$.

Each g-word of class 0 or 1 is nearly symmetric, and a standard class 2 g-word ($A^{p_1}B^{q_1}A^{p_2}B^{q_2}$) is nearly symmetric if and only if $p_1 = p_2$ or $q_1 = q_2$. We first show that Conjecture 1.3 is correct for class 2 words, in part because the technique generalizes in certain ways. We then describe necessary conditions for a word to be good (Theorems 3.1 and 4.1), thereby showing the rarity of such words. The idea is to produce PD matrices A and B for which the trace of a given word has nonzero imaginary part. Thus, not all eigenvalues could be positive.

2. Class 2 words. To prepare for the class 2 discussion and the general results that follow, some preliminaries are necessary.

DEFINITION 2.1. A *generalized polynomial* is an expression of the form

$$G(x_1, x_2, \dots, x_m) = \sum_{i=1}^{q} c_i \prod_{j=1}^{m} x_j^{p_{i,j}}$$

in which $c_i \in \mathbb{C}, p_{i,j} \in \mathbb{R}$, and the x_j are the variables.

A generalized polynomial (*g-poly*, for short) is said to be *reduced* if for each $i \neq t$, there is a j such that $p_{i,j} \neq p_{t,j}$. For example, $2x_1^0x_2^0 + x_1^{-2}x_2 + 3x_1x_2^0$ is a reduced g-polynomial, but $x_1^2x_2 - 3x_1x_2 + 5x_1^2x_2$ is not.

The proof in the class 2 case uses expressions that are generalized polynomials. They are also important in the study of larger class numbers. Let $\mathbb{R}_+^m = \{(x_1, x_2, ..., x_m) \mid x_j > 0,\ j = 1, \dots, m\}$ and let

$$R_G = \{(x_1, x_2, ..., x_m) \in \mathbb{R}_+^m \mid G(x_1, x_2, ..., x_m) = 0\},$$

the set of positive zeroes of G. We first write down a preliminary lemma for the one variable case.

LEMMA 2.2. If G is a reduced 1-variable ($m = 1$) g-poly and if 0 is an accumulation point for R_G, then $c_i = 0$ for all i.

Proof. Assume G is reduced with one variable x_1 and for some $i \in \{1, \dots, q\}$, $c_i \neq 0$. Also, suppose 0 is an accumulation point for R_G. Multiplying G by a large enough power of x_1, we can assume that G has only positive exponents – since this does not change R_G. Let $M = \min_i\{p_{i,1}\}$, and notice that

$$G = x_1^M \left(\sum_{i=1}^{q} c_i \, x_1^{p_{i,1}-M} \right) = x_1^M G_2.$$

Since G is reduced, so is G_2, and G_2 has a non-zero constant term. Also, since G_2 has the same set of positive zeroes as G, it follows that $R_{G_2} = R_G$. Now, 0 is an accumulation point for R_G, so there exists a sequence of $\lambda_r \in R_G$ $(r = 1, 2, \dots)$ such that $\lim_{r\to\infty} \lambda_r = 0$. Since, $G_2(\lambda_r) = 0$ for all r, we have that $0 = \lim_{r\to\infty} G_2(\lambda_r)$. But G_2 is continuous, and so $G_2(0) = 0$. This contradicts the fact that G_2 has a non-zero constant term, proving the lemma. $\square$

The lemma above allows us to prove the main observation we need about g-polys. We remark that this result is similar to one in [6, p.176] concerning (normal) polynomials over a field.

LEMMA 2.3. Let $S_1, \dots, S_m$ be infinite subsets of $\mathbb{R}_+$ with 0 being an accumulation point for each. If G is a reduced g-poly and if $G(a_1, \dots, a_m) = 0$ for all $a_j \in S_j$ $(j = 1, \dots, m)$, then $c_i = 0$ for all i.

Proof. For $m = 1$ and q arbitrary, we have Lemma 2.2 above. Therefore, we consider induction on m. Assume G is a reduced g-poly and for some $i \in \{1, \dots, q\}$, $c_i \neq 0$. Multiplying G by a large enough power of $\prod_{j=1}^m x_j$, we can assume that G has only positive exponents, as this does not change R_G. Let $M = \min_i \{p_{i,m}\}$, and examine

$$G = x_m^M \left(\sum_{i=1}^{q} c_i \, x_m^{p_{i,m}-M} \prod_{j=1}^{m-1} x_j^{p_{i,j}} \right) = x_m^M G_2.$$

Since G is reduced, so is G_2, and G_2 has non-zero terms that do not contain the variable x_m (i.e. those terms that only contain x_m^0). Specifically, let $F(x_1, \dots, x_{m-1})$ be the reduced g-poly in G_2 that does not contain the variable x_m. Since G_2 has the same set of positive zeroes as G, it follows that $R_{G_2} = R_G$. Now, fix $(a_1, \dots, a_{m-1}) \in S_1 \times \cdots \times S_{m-1}$ and examine the g-poly in 1 variable, $G_2(a_1, \dots, a_{m-1}, x_m)$. By Lemma 2.2, we must have that the constant term of this g-poly is zero. Whence, for all $(a_1, \dots, a_{m-1}) \in S_1 \times \cdots \times S_{m-1}$, it follows that $F(a_1, \dots, a_{m-1}) = 0$. By induction, each term in F must have zero coefficient, and this contradiction finishes the proof. $\square$

For the rest of the discussion, we will assume the following parameterization of A and B. Let $S = UU^T$ for some unitary matrix U, so that S is both unitary and symmetric. Then, we will assume

(2.1)
$$S = \begin{pmatrix} s_{1,1} & s_{2,1} & s_{3,1} \\ s_{2,1} & s_{2,2} & s_{3,2} \\ s_{3,1} & s_{3,2} & s_{3,3} \end{pmatrix}, \; A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & x_1 & 0 \\ 0 & 0 & y_1 \end{pmatrix}, \; E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & x_2 & 0 \\ 0 & 0 & y_2 \end{pmatrix}, \; B = SE\overline{S}$$

for $x_1, x_2, y_1, y_2 > 0$. We can view the trace of the g-word, W, under the assumption of (2.1) as

$$\operatorname{Tr}\left[A^{p_1} S E^{q_1} \overline{S} A^{p_2} S E^{q_2} \overline{S} \cdots A^{p_k} S E^{q_k} \overline{S}\right].$$

We are now ready to prove

THEOREM 2.4. A class 2 g-word is good if and only if it is nearly symmetric.

Proof. We may suppose that $W = A^{p_1} B^{q_1} A^{p_2} B^{q_2}$ is a class 2 g-word in standard form. If W is nearly symmetric, Theorem 1.2 shows that W is good. If W is not nearly symmetric, then we find a unitary matrix U and positive diagonal matrices A and E such that $B = SE\overline{S}$ gives W a non-real trace. By the above remark, the trace of W is that same as the trace of $A^{p_1} S E^{q_1} \overline{S} A^{p_2} S E^{q_2} \overline{S}$. Set $x = x_1 = x_2$, $y = y_1 = y_2$

and consider $A = \operatorname{diag}(1, x, y) = E$. Also, take U to be the unitary matrix

$$U = \frac{1}{4}\begin{pmatrix} 2 & -1-i & 3-i \\ -1+i & 3 & 1-2i \\ 3+i & 1+2i & -1 \end{pmatrix}.$$

With these assumptions, a straightforward computation reveals that the imaginary part of $\operatorname{Tr}[A^{p_1} S A^{q_1} \overline{S} A^{p_2} S A^{q_2} \overline{S}]$ is a g-poly in x and y given by $\frac{3}{128}$ times

$$\left[x^{p_2}\left(y^{p_1}-1\right)+x^{p_1}\left(1-y^{p_2}\right)+y^{p_2}-y^{p_1}\right]\cdot\left[x^{q_2}\left(y^{q_1}-1\right)+x^{q_1}\left(1-y^{q_2}\right)+y^{q_2}-y^{q_1}\right].$$

Now, fix $y > 1$ and suppose the above expression is 0 for all $x > 0$ (which is implied if W is good). Then, one of the factors has an accumulation point of 0 in its set of positive zeroes. Therefore, from Lemma 2.2, one of these factors is not reduced. In this case, we must have either $p_2 = p_1$ or $q_2 = q_1$. This completes the proof of the theorem. □

3. Good words are rare. We next show that the "density" of good words is 0, partly extending Theorem 2.4 in the direction of a proof of our conjecture for higher class words. We will prove that for good W there are certain non-trivial algebraic (actually linear) relations linking the p_i, q_i. If we view the space of good words (of class k) as a subset of $\mathbb{R}^{2k}$ parameterized by $\{(p_1, q_1, ..., p_k, q_k) \mid W \text{ is good}\}$, then it will follow that the set of good words is a set of measure zero in $\mathbb{R}^{2k}$. Consider a subset P of $\{p_1, \ldots, p_k\}$ (as variables) and similarly let Q be a subset of $\{q_1, \ldots, q_k\}$ (also as variables). Then, the full statement is given by

THEOREM 3.1. If $W = A^{p_1} B^{q_1} A^{p_2} B^{q_2} \cdots A^{p_k} B^{q_k}$ is good, then there exists a subset, $P \subseteq \{p_1, \ldots, p_k\}$, and a subset, $Q \subseteq \{q_1, \ldots, q_k\}$, such that

$$p_1 = \sum_{p \in P} p \quad \text{and} \quad q_1 = \sum_{q \in Q} q,$$

in which this pair of relations is not the trivial one,

$$p_1 = p_1 \quad \text{and} \quad q_1 = q_1.$$

COROLLARY 3.2. If the p_i are linearly independent over $\{-1, 0, 1\}$ and if the q_i are also linearly independent over $\{-1, 0, 1\}$, then W is bad.

As another immediate Corollary, we obtain Theorem 1.3 mentioned in the introduction.

We should remark that Theorem 3.1 gives another proof of Theorem 2.4. For in the case of class 2 words, we must have (since the $p_i, q_i \neq 0$) either $p_1 = p_2$ or $q_1 = q_2$ for W to be good. Before proving this theorem we need a few technical remarks. Assuming the parameterization as in (2.1), the trace of W can be viewed as a g-poly in x_1, x_2, y_1, and y_2 with exponents involving the p_i and q_i :

$$\operatorname{Tr}\left[A^{p_1} S E^{q_1} \overline{S} A^{p_2} S E^{q_2} \overline{S} \cdots A^{p_k} S E^{q_k} \overline{S}\right].$$

In fact, it is not hard to see that this trace will be a constant plus a (formal) sum of elements of the form,

$$c\, x_1^{\sum_{p\in P_1} p}\, y_1^{\sum_{p\in P_2} p}\, x_2^{\sum_{q\in Q_1} q}\, y_2^{\sum_{q\in Q_2} q}, \tag{3.1}$$

in which $c \in \mathbb{C}$, $P_1, P_2 \subseteq \{p_1, \ldots, p_k\}$, and $Q_1, Q_2 \subseteq \{q_1, \ldots, q_k\}$. Of course, here an empty sum is defined to be zero. We call an expression as above a *term* in the trace expansion of W. We will also say that p_i (q_i) is *contained* in a power of x_1, y_1 (x_2, y_2) if $p_i \in P_1, p_i \in P_2$ ($q_i \in Q_1, q_i \in Q_2$). As an example, consider $\mathrm{Tr}[A^{p_1}SE^{q_1}\overline{S}]$, corresponding to the g-word $W = A^{p_1}B^{q_1}$. This trace is

$$s_{11}\overline{s_{11}} + s_{21}\overline{s_{21}}x_2^{q_1} + s_{31}\overline{s_{31}}y_2^{q_1} + s_{21}\overline{s_{21}}x_1^{p_1} + s_{22}\overline{s_{22}}x_1^{p_1}x_2^{q_1} + s_{32}\overline{s_{32}}x_1^{p_1}y_2^{q_1}$$
$$+ s_{31}\overline{s_{31}}y_1^{p_1} + s_{32}\overline{s_{32}}x_2^{q_1}y_1^{p_1} + s_{33}\overline{s_{33}}y_2^{q_1}y_1^{p_1}.$$

Since these expressions are quite complicated (even for $k = 1$), we need a method of isolating the coefficients of individual terms as functions of the entries of S. The following lemma describes a way to determine these quantities.

LEMMA 3.3. Assume we have a representation (2.1). Consider an arbitrary term as in (3.1), and let $P = P_1 \cup P_2 = \{p_{i_1}, \ldots, p_{i_u}\}$ and $Q = Q_1 \cup Q_2 = \{q_{j_1}, \ldots, q_{j_v}\}$. So each element of P and Q is contained in a power of x_1, x_2, y_1, or y_2 in the given term of $\mathrm{Tr}[W] = \mathrm{Tr}[A^{p_1}SE^{q_1}\overline{S}A^{p_2}SE^{q_2}\overline{S}\cdots A^{p_k}SE^{q_k}\overline{S}]$. Then, this term will appear with the same coefficient in the trace of:

$$A^{p_{i_1}}SF\overline{S}FSF\overline{S}\cdots SE^{q_{j_1}}\overline{S}FS\cdots SE^{q_{j_v}}\overline{S}\cdots SF\overline{S}$$

where $F = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ replaces each instance of A^{p_i} (E^{q_j}) in which $p_i \notin P$ ($q_j \notin Q$).

Proof. Let $X_{1,1} = x_1^{p_1}, \ldots, X_{1,k} = x_1^{p_k}$; $X_{2,1} = x_2^{q_1}, \ldots, X_{2,k} = x_2^{q_k}$, and similarly, let $Y_{1,1} = y_1^{p_1}, \ldots, Y_{1,k} = y_1^{p_k}$; $Y_{2,1} = y_2^{q_1}, \ldots, Y_{2,k} = y_2^{q_k}$. Now, set

$$A_i = \begin{pmatrix} 1 & 0 & 0 \\ 0 & X_{1,i} & 0 \\ 0 & 0 & Y_{1,i} \end{pmatrix}, \quad E_i = \begin{pmatrix} 1 & 0 & 0 \\ 0 & X_{2,i} & 0 \\ 0 & 0 & Y_{2,i} \end{pmatrix}$$

for $i = 1, \ldots, k$ and examine the trace of

$$H = A_1SE_1\overline{S}A_2SE_2\overline{S}\cdots A_kSE_k\overline{S}.$$

This trace is a (normal) polynomial in $X_{1,i}$, $X_{2,i}$, $Y_{1,i}$, and $Y_{2,i}$. Next, consider the trace of

$$J = A_{i_1}SF\overline{S}FSF\overline{S}\cdots SE_{j_1}\overline{S}FS\cdots SE_{j_v}\overline{S}\cdots SF\overline{S},$$

where F as above replaces in H each instance of A_i (E_j) in which $p_i \notin P$ ($q_j \notin Q$). The trace of J is also a polynomial in $X_{1,i}$,$X_{2,i}$,$Y_{1,i}$,$Y_{2,i}$. But now, notice that if, for example, $p_i \notin P$, then every time a factor (when computing this trace) of $X_{1,i}$ would have appeared in $\mathrm{Tr}[H]$, it is replaced by a 0 – similarly for $X_{2,i}$,$Y_{1,i}$,$Y_{2,i}$. Thus, it is clear that $\mathrm{Tr}[J]$ has the desired term with the same coefficient as in $\mathrm{Tr}[H]$. ∎

Our first application of this result is the following.

LEMMA 3.4. Assuming that we have representation (2.1), the g-poly expression, $\mathrm{Tr}[A^{p_1}SE^{q_1}\overline{S}A^{p_2}SE^{q_2}\overline{S}\cdots A^{p_k}SE^{q_k}\overline{S}]$, has a real constant term.

Proof. Using Lemma 3.3, the constant term of the above trace is just the trace of: $\left(FSF\overline{S}\right)\left(FSF\overline{S}\right)\cdots\left(FSF\overline{S}\right) = \left(FSF\overline{S}\right)^k$. But

$$\left(FSF\overline{S}\right)^k = \begin{pmatrix} s_{1,1}\overline{s_{1,1}} & s_{1,1}\overline{s_{2,1}} & s_{1,1}\overline{s_{3,1}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^k$$

$$= \begin{pmatrix} \left(s_{1,1}\overline{s_{1,1}}\right)^k & s_{1,1}\overline{s_{2,1}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-1} & s_{1,1}\overline{s_{3,1}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-1} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Hence the trace of $A^{p_1}SE^{q_1}\overline{S}\cdots A^{p_k}SE^{q_k}\overline{S}$ has a real constant term, $\left(s_{1,1}\overline{s_{1,1}}\right)^k$. ∎

Call two exponents p_i and q_j *adjacent* if either $i = j$, $i-1 = j$, or $(i,j) = (1,k)$. For instance, p_2 and q_1 are adjacent. The following computation shows that we can always find terms with non-real coefficients.

LEMMA 3.5. Assuming (2.1) as before, the coefficient of any term, $x_1^{p_{i_1}}y_2^{q_{j_1}}$, in the trace of a class k word ($k > 1$) in which p_{i_1} and q_{j_1} are adjacent is given by:

$$\overline{s_{2,1}}s_{1,1}\overline{s_{3,1}}s_{3,2}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2} \quad \text{or} \quad s_{2,1}\overline{s_{1,1}}s_{3,1}\overline{s_{3,2}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2}.$$

Proof. First notice that we can assume we are dealing with the term $x_1^{p_1}y_2^{q_1}$ by (possibly) a reversal and (possibly) cycling. (A cycling is a similarity transformation, and a reversal corresponds to a conjugate transposition, which will only change the conjugacy of the coefficient). Therefore, we need only compute (by Lemma 3.3)

$$A^{p_1}SE^{q_1}\overline{S}FSF\overline{S}\cdots FSF\overline{S}.$$

This quantity can be represented compactly as:

$$A^{p_1}SE^{q_1}\overline{S}\left(FSF\overline{S}\right)^{k-1}.$$

A straightforward calculation gives us that the trace of the product of the two matrices $A^{p_1}SE^{q_1}\overline{S}$ and $\left(FSF\overline{S}\right)^{k-1}$ produces a coefficient of

$$\overline{s_{2,1}}s_{1,1}\overline{s_{3,1}}s_{3,2}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2}$$

for the $x_1^{p_1}y_2^{q_1}$ term as stated (and this term appears only once). Notice that this coefficient can be made non-real (for instance, using U as in the proof of Theorem 2.4). ∎

We are now ready to prove Theorem 3.1.

Proof of Theorem 3.1. Assuming the parameterization (2.1), notice that the imaginary part of $\mathrm{Tr}[W]$ is a g-poly in x_1, x_2, y_1, and y_2 with exponents involving the p_i and q_j. This g-poly has a term $x_1^{p_1} y_2^{q_1}$ with a nonzero coefficient by Lemma 3.5, and it is the only term of that form. By Lemma 2.3, if W is good, then this g-poly cannot be in a reduced form. Hence, there is some non-trivial relationship between the p_i, q_j. In other words, there exists a subset, $P \subseteq \{p_1, \ldots, p_k\}$, and a subset, $Q \subseteq \{q_1, \ldots, q_k\}$, such that

$$p_1 = \sum_{p \in P} p \quad \text{and} \quad q_1 = \sum_{q \in Q} q,$$

in which these equations do not both represent the trivial relations $p_1 = p_1$, $q_1 = q_1$. This proves the theorem. $\square$

4. Positive g-words. We next give a strong result for g-words with positive exponents, called *positive g-words.* For a class k g-word W in standard form, consider the list $L = L(W)$ of $2k$ real numbers:

$$L = \{p_1 + q_1,\ q_1 + p_2,\ p_2 + q_2,\ \ldots,\ p_k + q_k,\ q_k + p_1\},$$

the cyclically consecutive, pair-wise sums of the exponents. Enumerate the elements of L as $L_1 = p_1 + q_1,\ L_2 = q_1 + p_2,\ \ldots,\ L_{2k} = q_k + p_1$. Now, suppose that the minimum of L appears m times, and let $L_{i_1}, L_{i_2}, \ldots, L_{i_m}$ be the appearances of this minimum in L; of course, $\{i_1, \ldots, i_m\} \subseteq \{1, \ldots, 2k\}$.

Let $\#(L)_{\mathrm{o}}$ denote the number of i_r ($r = 1, \ldots, m$) that are odd, and let $\#(L)_{\mathrm{e}}$ denote the number of i_r that are even. For example, the word $W = A^4B^2A^3B^3A^4B^1$ has $L = \{6, 5, 6, 7, 5, 5\}$, and so $\#(L)_{\mathrm{o}} = 1$, $\#(L)_{\mathrm{e}} = 2$. We call a word *exact* if $\#(L)_{\mathrm{o}} = \#(L)_{\mathrm{e}}$. A word is *inexact* if it is not exact. We note combinatorially that nearly symmetric g-words are exact, but that there are exact g-words that are not nearly symmetric: $AB^2AB^3A^4B^5$. In a sense, exact words are a first order (linear) approximation to near symmetry. Of course, a class 2 g-word is nearly symmetric if and only if it is exact. We then have the following.

Theorem 4.1. All positive, good g-words are exact.

We should remark at this point that Theorems 3.1 and 4.1 are very different statements. For example, consider the word $W = A^1B^2A^2B^2A^3B^4$. In this case,

$$p_1 = p_1,\ q_1 = q_2;\quad p_2 = p_2,\ q_2 = q_1;\ \text{and}\quad p_3 = p_1 + p_2,\ q_3 = q_3$$

represent nontrivial pairs of relations. Thus, we cannot conclude that W is bad using only Theorem 3.1. However, from $L(W) = \{3, 4, 4, 5, 7, 5\}$, it follows that $\#(L)_{\mathrm{o}} = 1, \#(L)_{\mathrm{e}} = 0$, and so W is bad by Theorem 4.1.

Before we prove the theorem, we need a lemma that pertains only to positive g-words. It allows us to find positive semidefinite A and B for which $\mathrm{Tr}[W]$ is nonpositive instead of finding PD ones. It will then be enough to show the theorem for the following parameterization of the matrices A, B. As before let $S = UU^T$ for some unitary matrix U, but this time assume

$$S = \begin{pmatrix} s_{1,1} & s_{2,1} & s_{3,1} \\ s_{2,1} & s_{2,2} & s_{3,2} \\ s_{3,1} & s_{3,2} & s_{3,3} \end{pmatrix},\ A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & 0 \end{pmatrix},\ E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & y & 0 \\ 0 & 0 & 0 \end{pmatrix},\ B = SE\overline{S}, \tag{4.1}$$

for $x, y > 0$.

Lemma 4.2. Suppose there exist S, A, and E with the parameterization (4.1) that give a positive g-word, W, a nonzero imaginary part for its trace. Then, W is bad.

Proof. Assume that we have found an S, A, and E as above that give the positive g-word, W, a nonzero imaginary part for its trace. Given $\varepsilon > 0$, let W_ε denote the matrix product produced by replacing A with $A_\varepsilon = \mathrm{diag}(1, x, \varepsilon)$ and E with $E_\varepsilon = \mathrm{diag}(1, y, \varepsilon)$. We can, therefore, write $\mathrm{Tr}[W_\varepsilon]$ as the trace of:

$$A_\varepsilon^{p_1} S E_\varepsilon^{q_1} \overline{S} A_\varepsilon^{p_2} S E_\varepsilon^{q_2} \overline{S} \cdots A_\varepsilon^{p_k} S E_\varepsilon^{q_k} \overline{S}.$$

The imaginary part of this product will be the same as that of W except for an additional (possibly 0) expression involving sums of positive powers of ε. Since the imaginary part of W was assumed to be nonzero, by continuity, we can choose ε small enough so that this imaginary part stays nonzero. □

The trace, $\mathrm{Tr}[A^{p_1} S E^{q_1} \overline{S} \cdots A^{p_k} S E^{q_k} \overline{S}]$, of a word under the assumption of (4.1) can be viewed as a g-poly in x, y, with exponents involving the p_i and q_j. As before, it is not hard to see that this trace will be a constant plus a (formal) sum of terms of the form,

$$c\, x^{p_{i_1} + p_{i_2} + \cdots + p_{i_u}} y^{q_{j_1} + q_{j_2} + \cdots + q_{j_v}},$$

in which $c \in \mathbb{C}$, $\{p_{i_1}, \ldots, p_{i_u}\} \subseteq \{p_1, \ldots, p_k\}$, and $\{q_{j_1}, \ldots, q_{j_v}\} \subseteq \{q_1, \ldots, q_k\}$. Setting $y_1 = y_2 = 0$ in Lemma 3.3 above (which is a valid maneuver for positive g-words) gives us a method to determine the coefficients of such terms, and an argument similar to the one in Lemma 3.4 shows us that the constant term in this trace is real.

We next compute the coefficients that are attached to certain terms. The aim is to discover which terms can be made to have non-real coefficients. This will give us insight into what values of p_i and q_j guarantee that the word's trace can be made non-real. Our main result stems from the following.

Lemma 4.3. Assuming (4.1), let $P = \{p_{i_1}, \ldots, p_{i_u}\} \subseteq \{p_1, \ldots, p_k\}$ and let $Q = \{q_{j_1}, \ldots, q_{j_v}\} \subseteq \{q_1, \ldots, q_k\}$. Then, if the coefficient of the term

$$x^{p_{i_1} + p_{i_2} + \cdots + p_{i_u}} y^{q_{j_1} + q_{j_2} + \cdots + q_{j_v}}$$

is not real, there must be a $p_i \in P$ and a $q_j \in Q$ such that p_i and q_j are adjacent.

Proof. We will show the contrapositive. Let $P = \{p_{i_1}, \ldots, p_{i_u}\} \subseteq \{p_1, \ldots, p_k\}$ and let $Q = \{q_{j_1}, \ldots, q_{j_v}\} \subseteq \{q_1, \ldots, q_k\}$. Then, we prove that if there are no adjacent p_i, q_j in the P, Q, the coefficient of

$$x^{p_{i_1} + p_{i_2} + \cdots + p_{i_u}} y^{q_{j_1} + q_{j_2} + \cdots + q_{j_v}}$$

is real.

If both P and Q are empty, then there is nothing to show (the constant term is real). Next, notice that it suffices to prove the result under the assumption that $p_1 \in P$. This is because if $P \neq \emptyset$, we can perform an appropriate cycling (which will not change the coefficient) and relabel variables. And if $P = \emptyset$, an interchange (which swaps x, y) and a cycling will put our word into this form (all that will change is the conjugacy of the coefficient by our parameterization (4.1)). Using Lemma 3.3, it suffices to consider the matrix

$$J = A^{p_{i_1}} SF\overline{S}FSF\overline{S} \cdots SE^{q_{j_1}}\overline{S}FS \cdots SE^{q_{j_v}}\overline{S} \cdots SF\overline{S}$$

where F as in Lemma 3.3 replaces in

$$A^{p_1} SE^{q_1}\overline{S}A^{p_2}SE^{q_2}\overline{S} \cdots A^{p_k}SE^{q_k}\overline{S}$$

each instance of A^{p_i} (E^{q_j}) in which $p_i \notin P$ ($q_j \notin Q$). We will perform an induction on the class number k of a word, utilizing a special form of the matrices J.

Assume that for some k and for each P, Q with no adjacent elements, J has the form

$$\begin{pmatrix} * & * & * \\ s_{2,1}\overline{s_{1,1}}\, c_1 \cdot x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}} + g_1 & c_2 \cdot x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}} + g_2 & * \\ 0 & 0 & 0 \end{pmatrix}$$

where the constants c_1 and c_2 are real, $g_1 = g_1(x, y)$ and $g_2 = g_2(x, y)$ are g-polys, and the term

$$x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}}$$

doesn't appear in the (1,1) or (1,2) locations in the above matrix or in $g_1(x, y), g_2(x, y)$. Notice also that a matrix with the form described above has a trace in which a desired term has a real coefficient (namely, c_2).

The base case for our analysis will be $k = 1$. In this situation, the only term that doesn't violate the hypotheses about adjacency is x^{p_1}. A calculation reveals that,

$$A^{p_1}SF\overline{S} = \begin{pmatrix} s_{1,1}\overline{s_{1,1}} & s_{1,1}\overline{s_{2,1}} & s_{1,1}\overline{s_{3,1}} \\ x^{p_1}s_{2,1}\overline{s_{1,1}} & x^{p_1}s_{2,1}\overline{s_{2,1}} & x^{p_1}s_{2,1}\overline{s_{3,1}} \\ 0 & 0 & 0 \end{pmatrix}.$$

This matrix has the form given above and, thus, can be used as a base case for our induction.

We now proceed with the induction. Let k be given in which the lemma is true, and assume that we are given a class $k+1$ word and a pair P, Q with no adjacent elements. Then, the coefficient of the term,

$$x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}},$$

can be found by examining the matrix

$$J_1 = A^{p_{i_1}} SF\overline{S}FSF\overline{S} \cdots SE^{q_{j_1}}\overline{S}FS \cdots SE^{q_{j_v-1}}\overline{S} \cdots SF\overline{S}$$

involving k terms (originally looking like $A^{p_1}SE^{q_1}\overline{S} \cdots A^{p_k}SE^{q_k}\overline{S}$) multiplied by an appropriately transformed (using Lemma 3.3) $A^{p_{k+1}}SE^{q_{k+1}}\overline{S}$.

If $q_{k+1} \in Q$, then since $p_1 \in P$, p_1 and q_{k+1} would be adjacent, contrary to our assumption. Hence, we may assume $q_{k+1} \notin Q$. This leaves us with two cases: $p_{k+1} \in P$ or $p_{k+1} \notin P$.

Case 1: $p_{k+1} \notin P = \{p_{i_1}, \dots, p_{i_u}\}$.

By the inductive hypothesis, the expression J_1 above has the form:

$$\begin{pmatrix} * & * & * \\ s_{2,1}\overline{s_{1,1}}\, c_1 \cdot x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}} + g_1 & c_2 \cdot x^{p_{i_1}+\cdots+p_{i_u}} y^{q_{j_1}+\cdots+q_{j_v}} + g_2 & * \\ 0 & 0 & 0 \end{pmatrix}.$$

And since $p_{k+1} \notin P$, $q_{k+1} \notin Q$, we need only concern ourselves with the product of J_1 with $FSF\overline{S}$. From before, we know that

$$FSF\overline{S} \;=\; \begin{pmatrix} s_{1,1}\overline{s_{1,1}} & s_{1,1}\overline{s_{2,1}} & s_{1,1}\overline{s_{3,1}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Therefore, it is clear that $J_1 FSF\overline{S}$ preserves the special form of the matrix discussed in the inductive hypothesis.

Case 2: $p_{k+1} = p_{i_u} \in P$.

Since $p_{k+1} \in P$, we cannot have $q_k \in Q$ because then p_{k+1} and q_k would be adjacent. Therefore, we must have that the product

$$J_1 = A^{p_{i_1}} SF\overline{S} \cdots SE^{q_{j_1}}\overline{S}FS \cdots SE^{q_{j_v}}\overline{S} \cdots SF\overline{S},$$

involving k terms (originally looking like $A^{p_1}SE^{q_1}\overline{S} \cdots A^{p_k}SE^{q_k}\overline{S}$) complies with the induction hypothesis (the sets $P\backslash\{p_{k+1}\}$ and Q have no adjacent elements). Hence, we need only look at J_1 multiplied by the matrix, $A^{p_{i_u}}SF\overline{S}$, where by induction, J_1 looks like:

$$\begin{pmatrix} * & * & * \\ s_{2,1}\overline{s_{1,1}}\, c_1 \cdot x^{p_{i_1}+\cdots+p_{i_{u-1}}} y^{q_{j_1}+\cdots+q_{j_v}} + g_1 & c_2 \cdot x^{p_{i_1}+\cdots+p_{i_{u-1}}} y^{q_{j_1}+\cdots+q_{j_v}} + g_2 & * \\ 0 & 0 & 0 \end{pmatrix}.$$

A simple computation gives us

$$A^{p_{i_u}}SF\overline{S} = \begin{pmatrix} s_{1,1}\overline{s_{1,1}} & s_{1,1}\overline{s_{2,1}} & s_{1,1}\overline{s_{3,1}} \\ x^{p_{i_u}} s_{2,1}\overline{s_{1,1}} & x^{p_{i_u}} s_{2,1}\overline{s_{2,1}} & x^{p_{i_u}} s_{2,1}\overline{s_{3,1}} \\ 0 & 0 & 0 \end{pmatrix}.$$

As before, it is not too difficult to see that the new matrix produced, $J_1 A^{p_{i_u}}SF\overline{S}$, will preserve the special form needed for the induction. This completes the induction and the proof. □

We have shown above a necessary condition on a term for it to have a non-real coefficient. We need one more lemma to guarantee that there are some terms that that can be made to have non-real coefficients. This result is an analog of Lemma 3.5.

LEMMA 4.4. The coefficient of any term, $x^{p_{i_1}}y^{q_{j_1}}$ in a class k word ($k>1$) in which p_{i_1} and q_{j_1} are adjacent is given by:

$$\overline{s_{2,2}}\left(s_{2,1}\right)^2\overline{s_{1,1}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2} \quad \text{or} \quad s_{2,2}\left(\overline{s_{2,1}}\right)^2 s_{1,1}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2}.$$

Proof. We first notice that we can assume we are dealing with the term $x^{p_1}y^{q_1}$ by cycling and (possibly) a reversal. Therefore, by Lemma 3.3, we need only compute $A^{p_1}SE^{q_1}\overline{S}FSF\overline{S}\cdots FSF\overline{S}$. This is just $A^{p_1}SE^{q_1}\overline{S}\left(FSF\overline{S}\right)^{k-1}$. A straightforward calculation gives us,

$$\left(FSF\overline{S}\right)^{k-1} = \begin{pmatrix} \left(s_{1,1}\overline{s_{1,1}}\right)^{k-1} & s_{1,1}\overline{s_{2,1}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2} & s_{1,1}\overline{s_{3,1}}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Additionally, $A^{p_1}SE^{q_1}\overline{S}$ is

$$\begin{pmatrix} s_{1,1}\overline{s_{1,1}} + y^{q_1}s_{2,1}\overline{s_{2,1}} & s_{1,1}\overline{s_{2,1}} + y^{q_1}s_{2,1}\overline{s_{2,2}} & * \\ x^{p_1}\left(s_{2,1}\overline{s_{1,1}} + y^{q_1}s_{2,2}\overline{s_{2,1}}\right) & x^{p_1}\left(s_{2,1}\overline{s_{2,1}} + y^{q_1}s_{2,2}\overline{s_{2,2}}\right) & * \\ 0 & 0 & 0 \end{pmatrix}.$$

Therefore, taking the product of these two matrices and computing the trace gives us a coefficient of

$$s_{2,2}\left(\overline{s_{2,1}}\right)^2 s_{1,1}\left(s_{1,1}\overline{s_{1,1}}\right)^{k-2}$$

for the $x^{p_1}y^{q_1}$ term as stated. □

It should be clear that consecutive terms such as $x^{p_i}y^{q_i}$ and $x^{p_{i+1}}y^{q_i}$ have conjugate coefficients (by a reversal and cycling) and that these coefficients can, in fact, be made non-real (for example, using U again from the proof of Theorem 2.4).

We are now ready to prove Theorem 4.1.

Proof of Theorem 4.1. We will prove that an inexact word is bad. Take A, S, and E as in (4.1). As before, enumerate the elements of L as $L_1 = p_1 + q_1$, $L_2 = q_1 + p_2$, $\ldots$, $L_{2k} = q_k + p_1$. Now, suppose that the minimum of L appears m times, and let $L_{i_1}, L_{i_2}, \ldots, L_{i_m}$ be the appearances of this minimum in L. Without loss of generality, we suppose it is the one involving the two terms p_1 and q_1.

From Lemma 4.4, we know that the coefficients of these m terms can be made non-real for any class k word's trace. From Lemma 4.3, however, we also know that any other term that appears in the trace of $A^{p_1}B^{q_1}\cdots A^{p_k}B^{q_k}$ must contain two adjacent p_i, q_j in the exponents of x and y in order for it to have a non-real coefficient.

Set $x = y$, and notice that the imaginary part of the trace of an inexact word cannot be zero for all $x > 0$. This is because there are exactly m terms of the same minimum degree, $p_1 + q_1$ (since all of the p_i's and q_j's are positive), and they all have nonzero coefficients. From the discussion after Lemma 4.4, it follows that the sum of these coefficients (whose signs only alternate) is a non-zero constant times

$$\sum_{k=1}^{m}(-1)^{i_k} = \#\left(L\right)_{\mathrm{e}} - \#\left(L\right)_{\mathrm{o}}.$$

If the word is inexact, then by definition this sum will be non-zero. Therefore, taking x small enough, we can produce positive semidefinite Hermitian A and B that give W a non-real trace. This gives us positive definite A and B by Lemma 4.2, and concludes the proof of the theorem. $\square$

If a positive g-word W has $L(W)$ with $2k$ distinct elements, then there is only one minimum element in L. Hence, in this case W is inexact, and so Theorem 4.1 gives us the immediate fact.

COROLLARY 4.5. If W is a positive g-word and if $L(W)$ has distinct elements, then W is bad.

5. Remark. As a final remark, we note that we can prove Conjecture 1.3 for words of class 3 and 4. These proofs contain arguments similar to those in Theorem 2.4, however, they are much more cumbersome and do not shed any light on what is happening in general.

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