SUMS OF HERMITIAN SQUARES AS AN APPROACH TO THE BMV CONJECTURE

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Abstract. Lieb and Seiringer stated in their reformulation of the Bessis-Moussa-Villani conjecture that all coefficients of the polynomial $p(t) = \mathrm{tr}[(\mathrm{A}+\mathrm{B})^m]$ are nonnegative whenever A and B are any two positive semidefinite matrices of the same size. We will show that for all $m \in \mathbb{N}$ the coefficient of t^4 in $p(t)$ is nonnegative, using a connection to sums of Hermitian squares of non-commutative polynomials which has been established by Klep and Schweighofer. This implies by a famous result of Hillar that the coefficients of t^k are nonnegative for $0 \leq k \leq 4$.

1. Introduction

The Bessis-Moussa-Villani (BMV) conjecture, originally stated as a problem of quantum statistical mechanics, has a 30 year long history. Since its introduction in 1975 [1] many partial results have been given, see e.g. [13] for a review until 2000. The following reformulation of Lieb and Seiringer [12] is more capable to algebraic methods than the original one.

Conjecture 1.1 ((Bessis, Moussa, Villani)). *For all positive semidefinite matrices* A *and* B *and all* $m \in \mathbb{N}$*, the polynomial* $p(t) := \mathrm{tr}((\mathrm{A}+t\mathrm{B})^m) \in \mathbb{R}[t]$ *has only nonnegative coefficients.*

The coefficient of t^k in $p(t)$ for a given m is the trace of $S_{m,k}(\mathrm{A},\mathrm{B})$, where $S_{m,k}(\mathrm{A},\mathrm{B})$ is the sum of all words of length m in the letters A and B in which B appears exactly k times. For example $S_{4,2}(\mathrm{A},\mathrm{B}) = \mathrm{A}^2\mathrm{B}^2 + \mathrm{ABAB} + \mathrm{AB}^2\mathrm{A} + \mathrm{BABA} + \mathrm{B}^2\mathrm{A}^2 + \mathrm{BA}^2\mathrm{B}$.

In [1] it has already been shown that the BMV conjecture is true for 2×2 matrices. Since for $0 \leq k \leq 2$ or $m-2 \leq k \leq m$ each word in $S_{m,k}(\mathrm{A},\mathrm{B})$ has nonnegative trace, as is easily seen, the conjecture is true for $m \leq 5$. Hillar and Johnson [7] verified the first nontrivial case $m = 6, k = 3$ for positive semidefinite 3×3 matrices. Hägele [4] verified $m = 7$ which leads by a result of Hillar [6] to $m \leq 7$. Further, Klep and Schweighofer [9] derived that Conjecture 1.1 is true for $m \leq 13$. Whereas all these results fix m and consider arbitrary $k \leq m$, we take the opposite viewpoint, fix $k = 4$ and let $m \in \mathbb{N}$ be arbitrary. We will give a proof that

$$\mathrm{tr}(S_{m,4}(\mathrm{A},\mathrm{B})) \geq 0$$

with no restrictions on m or the matrix size of A and B.

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A result of Hillar [6] then implies that it is true for all $k \leq 4$ and arbitrary m, in particular if $k = 3$ which can't be shown directly by our method.

Using analytical methods, Fleischhack and Friedland [3] showed that for fixed positive semidefinite A, B and fixed k, the trace of $S_{m,k}(\mathrm{A},\mathrm{B})$ is nonnegative whenever m is big enough. Unfortunately, their lower bound on m is dependent of A and B. Otherwise this would imply the BMV conjecture.

To verify Conjecture 1.1 it is sufficient to show the nonnegativity of $\mathrm{tr}(S_{m,k}(\mathrm{A},\mathrm{B}))$ for any two positive semidefinite *real* matrices A and B of the same size. Since further every positive semidefinite real matrix A is decomposable as $\mathrm{A} = \mathrm{C}^2$ for some real matrix C we specify our examination to $S_{m,k}(\mathrm{C}^2,\mathrm{D}^2)$ where C and D are any two real symmetric matrices of the same size. To work in an algebraic context we identify $S_{m,k}(\mathrm{C}^2,\mathrm{D}^2)$ as a polynomial $S_{m,k}(X^2,Y^2)$ in two non-commuting variables X and Y.

For this let $\mathbb{R}\langle X,Y\rangle$ denote the unital associative $\mathbb{R}$-algebra freely generated by X and Y. The elements of $\mathbb{R}\langle X,Y\rangle$ are polynomials in the non-commuting variables X and Y with coefficients in $\mathbb{R}$. An element w of the monoid $\langle X,Y\rangle$, freely generated by X,Y, is called a *word* and $w_{(i)}$ its i-th letter. An element of the form aw, where $0 \neq a \in \mathbb{R}$ and $w \in \langle X,Y\rangle$, is called a *monomial* and a its *coefficient*. We endow $\mathbb{R}\langle X,Y\rangle$ with the involution $p \mapsto p^*$ fixing $\mathbb{R} \cup \{X,Y\}$ pointwise. In particular, for each word $w \in \langle X,Y\rangle$, w^* is its reverse. If $w^* = w$, w is called a *palindrome*. An element of the form g^*g for some $g \in \mathbb{R}\langle X,Y\rangle$ is called a *hermitian square*.

Using this terminology we define the polynomial $S_{m,k}(X,Y)$ as the polynomial in the variables X and Y as the sum of all monic monomials of total degree m and degree k in Y. Replacing X and Y by X^2 and Y^2 leads to the desired polynomial $S_{m,k}(X^2,Y^2)$, which results in $S_{m,k}(\mathrm{A},\mathrm{B})$ when we evaluate at symmetric matrices C and D, satisfying $\mathrm{C}^2 = \mathrm{A}$ and $\mathrm{D}^2 = \mathrm{B}$.

The invariance of the trace under cyclic permutations motivates the definition of cyclic equivalence [9]. A cyclic permutation of a word v of length m is a map σ, where $\sigma(v) = v_{(\sigma(1))}v_{(\sigma(2))}\cdots v_{(\sigma(m))}$, for which there exists some $k \in \mathbb{N}$ such that $\sigma(i) = i + k \mod m$ for all $i = 1,\ldots,m$. For example $v_{(1)}v_{(2)}v_{(3)} \mapsto v_{(3)}v_{(1)}v_{(2)}$ is a cyclic permutation whereas $v_{(1)}v_{(2)}v_{(3)} \mapsto v_{(3)}v_{(2)}v_{(1)}$ is not.

Definition 1.2. Two words $v,w \in \langle X,Y\rangle$ are called *cyclically equivalent* ($v \overset{\mathrm{cyc}}{\sim} w$) if $\sigma(v) = w$ for some cyclic permutation σ of v.

Two polynomials $f = \sum_w a_w w$ and $g = \sum_w b_w w$ with $a_w, b_w \in \mathbb{R}$ are cyclically equivalent if for each $v \in \langle X,Y\rangle$ the sums of coefficients of all words $w \in \langle X,Y\rangle$ which are cyclically equivalent to v are equal, i.e., $\sum_{w \overset{\mathrm{cyc}}{\sim} v} a_w = \sum_{w \overset{\mathrm{cyc}}{\sim} v} b_w$. This is equivalent to $f - g$ being a sum of commutators in $\mathbb{R}\langle X,Y\rangle$, where the commutator $[p,q]$ is defined by $[p,q] := pq - qp$.

The polynomials $f = X^2YX + YX^3 + 2X^2Y^2$ and $g = 2YX^3 + 2YX^2Y$ are cyclically equivalent since $f - g = [X^2, YX] + [2X^2Y, Y]$. Alternatively, the condition on the coefficients is easily checked as well.

Definition 1.3. The *order* ($\mathrm{ord}\, w$) of a word $w = w_{(1)}\cdots w_{(m)}$ of length m is the smallest positive integer k, such that $w_{(i+k)} = w_{(i)}$ for all $i = 1,\ldots,m$ where we identify $w_{(i+k)}$ with $w_{(i+k-m)}$ if $i + k > m$. Thus cyclically equivalent words have the same order. It can also be defined as the smallest integer $k \geq 1$ such that there exists a subword $v = v_{(1)}\cdots v_{(k)}$ of length k with $w = v\cdots v = v^{m/k}$. The equivalence of these two definitions follows easily by induction over the length of the subword v.

Remark 1.4. One obtains that the order of a word $w = v^{m/\operatorname{ord}(w)}$ in $S_{m,4}(X^2, Y^2)$ divides m. Further, since Y^2 appears the same number of times in every subword v, we get that $\frac{m}{\operatorname{ord}(w)}$ divides 4. In particular $\operatorname{ord}(w) \in \{m, \frac{m}{2}, \frac{m}{4}\} \cap \mathbb{N}$.

Our main result is the following.

Theorem 1.5. *For $k = 4$ and $m \in \mathbb{N}$ the polynomial $S_{m,4}(X^2, Y^2)$ is cyclically equivalent to a sum of Hermitian squares.*

Remark 1.6.
(i) Hägele [4] has shown that $S_{6,3}(X^2, Y^2)$ cannot be cyclically equivalent to a sum of Hermitian squares of a certain special form. Landweber and Speer generalized this result to $k = 3$ and $m \geq 6$ but $m \neq 11$ [10]. Using this result a fact of Klep and Schweighofer [9, Prop. 3.1] shows that $S_{m,3}(X^2, Y^2)$ cannot be cyclically equivalent to any sum of Hermitian squares if $m \geq 6$ and $m \neq 11$. Therefore we are interested in the case $k = 4$ and arbitrary $m \in \mathbb{N}$.
(ii) Since a sum of Hermitian squares is positive semidefinite on all real symmetric matrices, Theorem 1.5 implies that $\operatorname{tr}(S_{m,4}(A, B))$, the coefficient of t^4 in $p(t)$, for all $m \in \mathbb{N}$ is nonnegative for all positive semidefinite matrices A, B.

In the sequel we will present a proof of Theorem 1.5 by constructing a sum of Hermitian squares which is cyclically equivalent to $S_{m,4}(X^2, Y^2)$. By Remark 1.4 the order of words in $S_{m,4}(X^2, Y^2)$ divides m and 4. Thus, if m is odd all words in $S_{m,4}(X^2, Y^2)$ have order m, whereas in the even case order $\frac{m}{2}$ and $\frac{m}{4}$ are also possible. Therefore we split the proof in two parts, m odd and even, starting with the easier part, where m is odd.

2. Case m odd

To verify Theorem 1.5 it suffices to construct a sum of Hermitian squares f which is cyclically equivalent to $S_{m,4}(X^2, Y^2)$. Let m be fixed. Since $S_{m,4}(X^2, Y^2)$ is homogeneous in X and Y, one can reduce the set of words in a decomposition as sum of Hermitian squares, as in the commutative case, to the set of words of half the degree in X and Y. Thus we set

$$V = \{v \in \langle X, Y\rangle \mid \deg_X v = m - 4, \deg_Y v = 4\}.$$

Further we define the subsets

$$V_0 = \{v \in \{X^2, Y^2\}^{\frac{m-1}{2}} X \mid v = X^k Y^2 X^\ell Y^2 X^{k'+1}, k \leq k'\} \cap V,$$
$$V_1 = \{v \in X\{X^2, Y^2\}^{\frac{m-1}{2}} \mid v = X^{k+1} Y^2 X^\ell Y^2 X^{k'}, k + 1 \leq k'\} \cap V.$$

We denote the possible exponents of X in a word v_i by k_i, ℓ_i and k_i' such that for example every $v_i \in V_0$ is of the form $v_i = X^{k_i} Y^2 X^{\ell_i} Y^2 X^{k_i'+1}$ and satisfies the condition $k_i + \ell_i + k_i' = m - 5$ where $\ell_i, k_i, k_i' \in 2\mathbb{N}$ and $k_i \leq k_i'$.

The exponent k_i (respectively $k_i + 1$ if $v_i \in V_1$) is bounded by d, the highest possible even (respectively odd) number which is less than or equal to $\frac{m-5}{2}$, thus the maximum of these bounds is in any case $\frac{m-5}{2}$.

Now, we will construct a sum of Hermitian squares f. For given $k \in \mathbb{N}$ let $k(2)$ denote the remainder of k modulo 2. Then we group the words $v_i \in V_0$ (respectively

V_1) according to k_i. For every $k = 0, 1, 2, \dots, \frac{m-5}{2}$ we add all words $v_i \in V_{k(2)}$ with $k_i + k(2) = k$ and obtain a polynomial f_k. By construction all words in $f_k^* f_k$ have even exponents in X and Y. Finally, we set

$$f := m \sum_{k=0}^{\frac{m-5}{2}} f_k^* f_k. \tag{1}$$

Example 2.1. (a) $m = 7$: We have $V_0 = \{Y^2X^2Y^2X, Y^4X^3\}$ and $V_1 = \{XY^4X^2\}$ which leads to

$$f_0 = Y^2X^2Y^2X + Y^4X^3 \quad \text{and} \quad f_1 = XY^4X^2$$

and finally

$$\begin{aligned} S_{7,4}(X^2, Y^2) &\overset{\text{cyc}}{\sim} 7\,(f_0^* f_0 + f_1^* f_1) \\ &= 7(XY^2X^2Y^4X^2Y^2X + XY^2X^2Y^6X^3 + X^3Y^6X^2Y^2X + X^3Y^8X^3 \\ &\quad + XY^4X^4Y^4X). \end{aligned}$$

This representation is of the same kind as the one given by Hägele in [4].

(b) $m = 9$: Since $V_0 = \{Y^2X^2Y^2X^3, Y^4X^5, X^2Y^4X^3, Y^2X^4Y^2X\}$ and $V_1 = \{XY^4X^4, XY^2X^2Y^2X^2\}$ we get by construction

$$\begin{aligned} f_0 &= Y^2X^2Y^2X^3 + Y^4X^5 + Y^2X^4Y^2X, \\ f_1 &= XY^2X^2Y^2X^2 + XY^4X^4 \quad \text{and} \\ f_2 &= X^2Y^4X^3. \end{aligned}$$

One easily checks $S_{9,4}(X^2, Y^2) \overset{\text{cyc}}{\sim} 9\,(f_0^* f_0 + f_1^* f_1 + f_2^* f_2)$.

We will prove that f is the desired sum of Hermitian squares in two steps. First all words appearing in f will be shown to be pairwise cyclically inequivalent. By construction each word in f appears in $S_{m,4}(X^2, Y^2)$ and has order m. Since up to cyclic equivalence each word in $S_{m,4}(X^2, Y^2)$ appears m times, it suffices to show that the sums of coefficients in both polynomials are the same.

Remark 2.2. To compare two words appearing in f with respect to cyclic equivalence we use the following method. Since Y^2 appears exactly four times in each word w of f, we know $w = X^{n_0}Y^2X^{n_1}Y^2X^{n_2}Y^2X^{n_3}Y^2X^{n'_4}$ for some $n_0, \dots, n_3, n'_4$. Further w is cyclically equivalent to $\tilde{w} := Y^2X^{n_1}Y^2X^{n_2}Y^2X^{n_3}Y^2X^{n_4}$ where $n_4 = n'_4 + n_0$, i.e. $\tilde{w}$ consists of four groups $Y^2X^{n_i}$. Let w' be another word with exponents m_i, i.e., $\tilde{w}' := Y^2X^{m_1}Y^2X^{m_2}Y^2X^{m_3}Y^2X^{m_4}$. Then $\tilde{w}$ and $\tilde{w}'$ are the same or $n_i = m_{i-j}$ ($i - j \mod 4$) for $i = 1, \dots, 4$ and $j = 1, 2, 3$, which can be obtained by "rotating" $\tilde{w}'$ j times, i.e., for $j = 1$ one shifts the first group $Y^2X^{m_1}$ to the end, for $j = 2$ one shifts also the second group to the end and so on, thus m_i becomes m_{i-j}.

For simplicity we use the fact that rotating three times is the same as rotating once in the reverse direction, i.e., shifting the group $Y^2X^{m_4}$ to the beginning. Thus rotating w' three times is the same as fixing w' and rotating w once. Therefore we can omit $j = 3$ by symmetry.

Lemma 2.3. *All words appearing in f are pairwise cyclically inequivalent.*

Proof. By construction a word w in f is either a word in $\sum_{2k} f_{2k}^* f_{2k}$ thus of the form $w = v_1^* v_2$ where $v_1, v_2 \in V_0$ and $k_1 = k_2$, i.e.,

$$w = X^{k_1'+1} Y^2 X^{\ell_1} Y^2 X^{2k_1} Y^2 X^{\ell_2} Y^2 X^{k_2'+1} \overset{\text{cyc}}{\sim} Y^2 X^{\ell_1} Y^2 X^{2k_1} Y^2 X^{\ell_2} Y^2 X^{k_1'+k_2'+2}.$$

Or it is a word in $\sum_{2k} f_{2k+1}^* f_{2k+1}$ thus of the form $w = v_1^* v_2$ where $v_1, v_2 \in V_1$ and $k_1 = k_2$. The same is true for any other word $w' = v_3^* v_4$. As is easily seen $\tilde{w} = \tilde{w}'$ is only possible if $v_1 = v_3$ and $v_2 = v_4$. We are left with the following cases.

If w and w' are words in $\sum_{2k} f_{2k}^* f_{2k}$ which are cyclically equivalent then we have to consider

(a) $\ell_1 = 2k_3, \quad 2k_1 = \ell_4, \quad \ell_2 = k_3' + k_4' + 2, \quad k_1' + k_2' + 2 = \ell_3$ or
(b) $\ell_1 = \ell_4, \quad 2k_1 = k_3' + k_4' + 2, \quad \ell_2 = \ell_3, \quad k_1' + k_2' + 2 = 2k_3$.

In (a) $2k_3 + k_1 + k_1' = \ell_1 + k_1 + k_1' = \ell_3 + k_3 + k_3' = k_1' + k_2' + 2 + k_3 + k_3'$ leads to $k_1 + k_3 = k_2' + k_3' + 2$ contradicting $k_1 + k_3 \le k_2' + k_3' < k_2' + k_3' + 2$. Subcase (b) leads to $2k_1 = k_3' + k_4' + 2 > 2k_3 = k_1' + k_2' + 2 > 2k_1$, which is not possible.

The case that w, w' are words in $\sum_{2k} f_{2k+1}^* f_{2k+1}$ works the same way.

If w is a word in $\sum_{2k} f_{2k}^* f_{2k}$ and w' a word in $\sum_{2k} f_{2k+1}^* f_{2k+1}$, then we have

(a) $\ell_1 = k_3' + k_4', \quad 2k_1 = \ell_3, \quad \ell_2 = 2k_3 + 2, \quad k_1' + k_2' + 2 = \ell_4$ or
(b) $\ell_1 = \ell_3, \quad 2k_1 = 2k_3' + 2, \quad \ell_2 = \ell_4, \quad k_1' + k_2' + 2 = k_3' + k_4'$.

In (a) $k_3' + k_4' + k_1 + k_1' = \ell_1 + k_1 + k_1' = \ell_3 + k_3 + k_3' = 2k_1 + k_3 + k_3'$ leads to $k_1' + k_4' = k_1 + k_3 = k_1 + k_4 < k_1' + k_4'$. Subcase (b) contradicts $k_1, k_3' \in 2\mathbb{N}$.

If w is a word in $\sum_{2k} f_{2k+1}^* f_{2k+1}$ and w' in $\sum_{2k} f_{2k}^* f_{2k}$, we exchange w and w'.

Summarizing, despite the trivial case that w and w' are constructed by the same subwords v_i, they cannot be cyclically equivalent. □

Thus every word in f has its order m as coefficient. Since up to cyclic equivalence this is the same in $S_{m,4}(X^2, Y^2)$, we are done by the following lemma.

Lemma 2.4. *The number of pairwise cyclically inequivalent words in f is the same as in $S_{m,4}(X^2, Y^2)$.*

Proof. $S_{m,4}(X^2, Y^2)$ contains $\binom{m}{4}$ words. Since each word has order m, there are

$$\frac{1}{m}\binom{m}{4} = \frac{1}{6}\left(\frac{m-3}{2}\right)\left(\frac{m-1}{2}\right)(m-2)$$

pairwise cyclically inequivalent words in $S_{m,4}(X^2, Y^2)$.

Let $k \in \mathbb{N}$ be fixed. Then f_k consists of $\frac{m-3}{2} - k$ different words. For example, if k is even then there are $\frac{1}{2}(m - 5 - k_1) + 1$ possibilities for $k_1, \ell_1, k_1' \in 2\mathbb{N}$ with $\ell_1 + k_1' = m - 5 - k_1$ (namely $k_1' = m - 5 - k_1 - \ell_1, \ell_1 = 0, 2, \ldots m - 5 - k_1$), the restriction $k_1 \le k_1'$ of V_0 excludes $\frac{k_1}{2}$ possibilities.

Thus the number of words in f is given by

$$\sum_{k=0}^{\frac{m-5}{2}} \left(\frac{m-3}{2} - k\right)^2 = \sum_{k=0}^{\frac{m-3}{2}} k^2 = \frac{1}{6}\left(\frac{m-3}{2}\right)\left(\frac{m-1}{2}\right)(m-2).$$

□

Remark 2.5. After we had finished the proof of this case, we heard of the recent work of Landweber and Speer [10] who proved the same result (for odd m) by quite similar techniques; but they haven't investigated the case where m is even. They found a sum of Hermitian squares which only consists of words w in

$$V_2 := \{v \in X\{X^2, Y^2\}^{\frac{m-1}{2}} \mid v = X^{k+1}Y^2X^lY^2X^{k'}\} \cap V.$$

Let $v_i = w_iX \in V_0$ for $i = 1, 2$. Starting with f and using

$$v_1^*v_2 = (Xw_1)^*Xw_2 = w_1^*XXw_2 \overset{\text{cyc}}{\sim} Xw_2w_1^*X = (w_2^*X)^*(w_1^*X) = (v_2^*)^*(v_1^*)$$

and $V_1 \subseteq V_2$ leads to a sum of Hermitian squares $\tilde{f}$ which is exactly the representation found by Landweber and Speer.

This result agrees with the more general Proposition 3.1 in [9] which in particular states that independent of k in the case m odd once one has found a representation as sum of Hermitian squares one can also find a representation using only of words of V_2.

3. Case m even

Since words in $S_{m,4}(X^2, Y^2)$ now have order m, $\frac{m}{2}$ or $\frac{m}{4}$, the constructed polynomial f of the last section is further not cyclically equivalent to $S_{m,4}(X^2, Y^2)$. Thus we will add weights on the words in our construction to respect the different orders.

Let m be fixed and $V = \{v \in \langle X, Y\rangle \mid \deg_X v = m - 4, \deg_Y v = 4\}$. Further we define the subsets

$$V_0 = \{v \in \{X^2, Y^2\}^{\frac{m}{2}} \mid v = X^kY^2X^\ell Y^2X^{k'}, k \le k'\} \cap V,$$
$$V_1 = \{v \in X\{X^2, Y^2\}^{\frac{m-2}{2}}X \mid v = X^{k+1}Y^2X^\ell Y^2X^{k'+1}, k \le k'\} \cap V.$$

To distinguish even and odd exponents, we define $\hat{k}_i := k_i + 1$ and $\hat{k}_i' := k_i' + 1$. Then every $v_i \in V_0$ is of the form $v_i = X^{k_i}Y^2X^{\ell_i}Y^2X^{k_i'+1}$ and satisfies $k_i + \ell_i + k_i' = m - 4$ where $\ell_i, k_i, k_i' \in 2\mathbb{N}$ and $k_i \le k_i'$, whereas every $v_i \in V_1$ satisfies $\hat{k}_i + \ell_i + \hat{k}_i' = m - 4$. Thus the maximal possible exponent k_i respectively $\hat{k}_i$ (if m is not divisible by 4) is given by $\frac{m-4}{2}$.

Now we construct our desired sum of Hermitian squares as follows. Let $k \in \mathbb{N}$ and let $k(2)$ denote the remainder of k modulo 2. For every $k = 0, 1, 2, \dots \frac{m-4}{2}$ we add all words $v_i \in V_{k(2)}$ with $k_i + k(2) = k$ as in the case where m is odd, but we weight the words with $k_i < k_i'$ with coefficient 1 and the words with $k_i = k_i'$ with coefficient $\frac{1}{2}$. This leads to a polynomial f_k which contains exactly one word with coefficient $\frac{1}{2}$ whereas all other coefficients are 1. Finally we set

$$f := m \sum_{k=0}^{\frac{m-4}{2}} f_k^* f_k. \tag{2}$$

Example 3.1. $m = 8$: We have $V_0 = \{Y^2X^2Y^2X^2, Y^4X^4, X^2Y^4X^2, Y^2X^4Y^2\}$ and $V_1 = \{XY^4X^3, XY^2X^2Y^2X\}$ which leads to

$$f_0 = Y^2X^2Y^2X^2 + Y^4X^4 + \frac{1}{2}Y^2X^4Y^2$$
$$f_1 = XY^4X^3 + \frac{1}{2}XY^2X^2Y^2X \quad \text{and}$$
$$f_2 = \frac{1}{2}X^2Y^4X^2.$$

Then one easily verifies $S_{8,4}(X^2,Y^2) \overset{\text{cyc}}{\sim} 8(f_0^*f_0 + f_1^*f_1 + f_2^*f_2)$.

Now for example the words $w = (Y^2X^2Y^2X^2)^*(Y^2X^4Y^2)$ in $f_0^*f_0$ and $w' = (XY^2X^2Y^2X)^*(XY^4X^3)$ in $f_1^*f_1$ are cyclically equivalent but due to our weights their coefficients sum up to $\operatorname{ord}(w) = 8$.

The proof of cyclic equivalence works similarly as in the case where m is odd. But since there are now cyclically equivalent words appearing in f, we have to calculate more carefully. We will show first that the sum of coefficients of cyclically equivalent words in f is less than or equal to their order. Since each word in f appears in $S_{m,4}(X^2,Y^2)$ we will finish by showing that the sums of coefficients are equal in both representations.

Lemma 3.2. *The sum of coefficients of cyclically equivalent words in f is less than or equal to the order of the corresponding words.*

Proof. We will use the same method as explained in Remark 2.2 of the last section. Let w, w' be two different words appearing in f and $w \overset{\text{cyc}}{\sim} w'$.

If w and w' are words in $\sum f_{2k}^* f_{2k}$. Then either w and w' are equal or one of the following subcases holds:

(a) $\ell_1 = 2k_3, \quad 2k_1 = \ell_4, \quad \ell_2 = k_3' + k_4', \quad k_1' + k_2' = \ell_3$
(b) $\ell_1 = \ell_4, \quad 2k_1 = k_3' + k_4', \quad \ell_2 = \ell_3, \quad k_1' + k_2' = 2k_3$

In subcase (a) we obtain $k_3 + k_1 = k_2' + k_3'$ from $2k_3 + k_1 + k_1' = \ell_1 + k_1 + k_1' = \ell_3 + k_3 + k_3' = k_1' + k_2' + k_3 + k_3'$, thus $k_1 = k_2'$ and $k_3 = k_3'$. Further we obtain from $\ell_1 + k_1 + k_1' = \ell_4 + k_3 + k_4'$ that $k_1' - k_1 = k_4' - k_3$. In (b) we obtain $2k_1 = k_3' + k_4' \geq 2k_3 = k_1' + k_2' \geq 2k_1$, thus equality holds, which leads to $w = w'$.

The other cases work in the same way by replacing k_i by $\hat{k}_i$ whenever w is a word in $\sum f_{2k+1}^* f_{2k+1}$ and k_i' respectively if w' is a word in $\sum f_{2k+1}^* f_{2k+1}$. If w and w' are not in the same set $\sum f_{2k}^* f_{2k}$ or $\sum f_{2k+1}^* f_{2k+1}$, then they obviously cannot be equal.

Summarizing, we derife that when $w \overset{\text{cyc}}{\sim} w'$ but $w \neq w'$ then $k_1 = k_2'$, $k_3 = k_3'$ and $k_1' - k_1 = k_4' - k_3$ or by symmetry (confer Remark 2.2) $k_3 = k_4'$, $k_1 = k_1'$ and $k_3' - k_3 = k_2' - k_1$ holds, where the first set of equations describes the words which differ by one rotation, and the second set describes the case of three rotations.

Assuming, there are two different words w', w'' both cyclically equivalent to w. Then all three are pairwise cyclically equivalent and at least two of them (for example w', w'') are in $\sum_k f_k^* f_k$ (k even or odd). Thus each of them satisfies one set of equations, but then w' and w'' differ by two rotations, which leads to equality (subcase (b)). Therefore there are at most two words in f which are pairwise cyclically equivalent.

To conclude the proof, if $w = v_1^* v_2$ with $k_1 = k_1' = k_2 = \frac{m-4}{4}'$ then $\ell_1 = m - 4 - 2k_1 = \frac{m-4}{2} = \ell_2$, thus w has order $\frac{m}{4}$ which is equal to the coefficient of w in f. A cyclically equivalent word $w' = v_3^* v_4$ has to satisfy $k_3 = k_3' = k_4'$ and $2k_3 = \ell_1 = 2k_1$ which leads to $w = w'$. Therefore there is no other word $w' \overset{\text{cyc}}{\sim} w$ in f. In all other cases the coefficient of w is half of the order of w. Since there are at most two pairwise cyclically equivalent words we are done. □

Lemma 3.3. *The sum of coefficients in both polynomials is the same.*

Proof. The sum of coefficients in $S_{m,4}(X^2,Y^2)$ is $\binom{m}{4} = \frac{1}{24} m(m-1)(m-2)(m-3)$.

For every $k = 0, 1, 2 \ldots, \frac{m-4}{2}$ each polynomial f_k has one word with coefficient $\frac{1}{2}$ and $\frac{m-4}{2} - k$ times coefficient 1. Thus the sum of coefficients in f is given by

$$m \sum_{k=0}^{\frac{m-4}{2}} \Big(\frac{m-4}{2} - k + \frac{1}{2}\Big)^2 = \frac{m(m-2)}{8} + m \sum_{k=0}^{\frac{m-4}{2}} (k^2 + k)$$
$$= \frac{m}{24}\big(3(m-2) + (m-4)(m-2)m\big) = \frac{1}{24} m(m-1)(m-2)(m-3).$$

□

4. Concluding Remarks

(a) To get an idea how sums of Hermitian squares which are cyclically equivalent to $S_{m,4}(X^2, Y^2)$ might look like, we used numerical computations extending those done by Klep and Schweighofer [9]. In particular we used NCAlgebra [8], YALMIP [11] and SeDuMi [14] as the starting point of our investigation.

(b) As in the case m odd one might consider $V_2 = \{v \in \{X^2, Y^2\}^{\frac{m}{2}}\} \cap V$ if m is even. Then one can find a much more complicated sum of Hermitian squares which is cyclically equivalent to $S_{m,4}(X^2, Y^2)$ and consists just of words in V_2 if $m(4) = 2$, i.e., m is even but not divisible by 4.

Since all words are words in the letters X^2 and Y^2 one obtains by substitution that $S_{m,4}(X, Y)$ is cyclically equivalent to a sum of Hermitian squares, which implies $\mathrm{tr}(S_{m,4}(\mathrm{A}, \mathrm{B})) \geq 0$ for *all* real Hermitian matrices A, B of the same size. This result has recently, independently been found by Collins, Dykema and Torres-Ayala [2].

(c) Landweber and Speer [10] showed that despite a few exceptions (which all have been solved) one cannot find a representation of $S_{m,k}(X^2, Y^2)$ as a sum of Hermitian squares if m or k is odd. But they have no negative results if m and k are both even. This gap has recently been filled by Collins, Dykema and Torres-Ayala [2] who proved that, despite the case (16,8), $S_{m,k}(X^2, Y^2)$ is not cyclically equivalent to a sum of Hermitian squares if $m - 6 \geq k \geq 6$ and $m \geq 16$. Thus this approach cannot proof the BMV conjecture.

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