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Kyoto University
Extensions of the BMV-conjecture

Frank Hansen

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Abstract

The Bessis-Moussa-Villani conjecture asserts that for any $n \times n$ matrices $A$ and $B$ such that $A$ is Hermitian and $B$ is positive semi-definite, the function $t \rightarrow \text{Tr} \exp(A - tB)$ is the Laplace transform of a positive measure. We say that a function $f$, defined on the positive half-line, has the BMV-property if for arbitrary $n \times n$ matrices $A$ and $B$ such that $A$ is positive definite and $B$ is positive semi-definite, the function $t \rightarrow \text{Tr} f(A + tB)$ is the Laplace transform of a positive measure. The BMV-conjecture is thus equivalent to the assertion that the function $t \rightarrow \exp(-t)$ has the BMV-property.

We prove that any non-negative and operator monotone decreasing function defined on the positive half-line has the BMV-property.

Key words: Trace functions, BMV-conjecture.

1 Introduction

Studying perturbations of exactly solvable Hamiltonian systems in statistical mechanics Bessis, Moussa and Villani [2] noted that the Padé approximant to the partition function $Z(\beta) = \text{Tr} \exp(-\beta(H_0 + \lambda H_1))$ may be efficiently calculated, if the function

$$
\lambda \rightarrow \text{Tr} \exp(-\beta(H_0 + \lambda H_1))
$$

is the Laplace transform of a positive measure. The authors then noted that this is indeed true for a system of spinless particles with local interactions bounded from below. The statement also holds if $H_0$ and $H_1$ are commuting operators, or if they are just $2 \times 2$ matrices. These observations led to the formulation of the following conjecture:
Conjecture (BMV). Let $A$ and $B$ be $n \times n$ matrices for some natural number $n$, and suppose that $A$ is self-adjoint and $B$ is positive semi-definite. Then there is a positive measure $\mu$ with support in the closed positive half-axis such that

$$\text{Tr} \exp(A - tB) = \int_0^\infty e^{-st} d\mu(s)$$

for every $t \geq 0$.

The Bessis-Moussa-Villani (BMV) conjecture may be reformulated as an infinite series of inequalities.

Theorem (Bernstein). Let $f$ be a real $C^\infty$-function defined on the positive half-axis. If $f$ is completely monotone, that is

$$(-1)^n f^{(n)}(t) \geq 0 \quad t > 0, \; n = 0, 1, 2, \ldots,$$

then there exists a positive measure $\mu$ on the positive half-axis such that

$$f(t) = \int_0^\infty e^{-st} d\mu(s)$$

for every $t > 0$.

The BMV-conjecture is thus equivalent to saying that the function

$$f(t) = \text{Tr} \exp(A - tB) \quad t > 0$$

is completely monotone. A proof of Bernstein's theorem can be found in [4].

Assuming the BMV-conjecture one may derive a similar statement for free semicircularly distributed elements in a type $II_1$ von Neumann algebra with a faithful trace. This consequence of the conjecture has been proved by Fannes and Petz [6]. A hypergeometric approach by Drmota, Schachermayer and Teichmann [5] gives a proof of the BMV-conjecture for some types of $3 \times 3$ matrices. This paper is a review article based on [10].

1.1 Equivalent formulations

The BMV-conjecture can be stated in several equivalent forms.

Theorem 1.1. The following conditions are equivalent:

(i). For arbitrary $n \times n$ matrices $A$ and $B$ such that $A$ is self-adjoint and $B$ is positive semi-definite the function $f(t) = \text{Tr} \exp(A - tB)$, defined on the positive half-axis, is the Laplace transform of a positive measure supported in $[0, \infty)$. 

(ii). For arbitrary $n \times n$ matrices $A$ and $B$ such that $A$ is self-adjoint and $B$ is positive semi-definite the function $g(t) = \text{Tr} \exp(A + tB)$, defined on the positive half-axis, is of positive type.

(iii). For arbitrary positive definite $n \times n$ matrices $A$ and $B$ the polynomial $P(t) = \text{Tr}(A + tB)^p$ has non-negative coefficients for any $p = 1, 2, \ldots$.

(iv). For arbitrary positive definite $n \times n$ matrices $A$ and $B$ the function $\varphi(t) = \text{Tr} \exp(A + tB)$ is $m$-positive on some open interval of the form $(-\alpha, \alpha)$.

The first statement is the BMV-conjecture, and it readily implies the second statement by analytic continuation. The sufficiency of the second statement is essentially Bochner's theorem. The implication $(iii) \Rightarrow (i)$ is obtained by applying Bernstein's theorem and approximation of the exponential function by its Taylor expansion. The implication $(i) \Rightarrow (iii)$ was proved by Lieb and Seiringer [16]. A function $\varphi : (-\alpha, \alpha) \to \mathbb{R}$ is said to be $m$-positive, if for arbitrary self-adjoint $k \times k$ matrices $X$ with non-negative entries and spectra contained in $(-\alpha, \alpha)$ the matrix $\varphi(X)$ has non-negative entries. The implication $(iii) \Rightarrow (iv)$ follows by approximation, while the implication $(iv) \Rightarrow (i)$ follows by Bernstein's theorem and [8, Theorem 3.3] which states that an $m$-positive function is real analytic with non-negative derivatives in zero.

In a recent paper [13] Hillar studied the coefficients of the above polynomial $P(t) = \text{Tr}(A + tB)^p$. The coefficient of $t^k$ in $P(t)$ is the trace of the so-called $k$th Hurwitz product $S_{p,k}(A, B)$ of $A$ and $B$, which is the sum of all words of length $p$ in $A$ and $B$ in which $B$ appears $k$ times. This polynomial has real coefficients, and in [15] it is proved that each constituent word in $S_{p,k}(A, B)$ has positive trace for $p < 6$ and all $n$. The first case in which the conjecture is in doubt is thus for $n = 3$ and $p = 6$. Even in this case all coefficients except $\text{Tr} S_{6,3}(A, B)$ were known to be positive. The question is very subtle since some of the words in the Hurwitz product may have negative trace. It was shown in [15] that the word $ABABBA$ may have negative trace for some positive definite $3 \times 3$ matrices $A$ and $B$. Finally it was proved in [14], using heavy computation, that the polynomial $P(t)$ has positive coefficients\footnote{This means that the non-zero coefficients of the polynomial are positive.} also in the case $n = 3$ and $p = 6.$
2 Preliminaries and main result

Let $f$ be a real function of one variable defined on a real interval $I$. We consider for each natural number $n$ the associated matrix function $x \rightarrow f(x)$ defined on the set of self-adjoint matrices of order $n$ with spectra in $I$. The matrix function is defined by setting

$$f(x) = \sum_{i=1}^{p} f(\lambda_i)P_i \quad \text{where} \quad x = \sum_{i=1}^{p} \lambda_i P_i$$

is the spectral resolution of $x$. The matrix function $x \rightarrow f(x)$ is Fréchet differentiable [7] if $I$ is open and $f$ is continuously differentiable [3].

2.1 The BMV-property

Definition 2.1. A function $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is said to have the BMV-property, if to each $n = 1, 2, \ldots$ and each pair of $n \times n$ matrices $A$ and $B$, such that $A$ is positive definite and $B$ is positive semi-definite, there is a positive measure $\mu$ with support in $[0, \infty)$ such that

$$\text{Tr} f(A + tB) = \int_{0}^{\infty} e^{-st} d\mu(s)$$

for every $t > 0$.

The BMV-conjecture is thus equivalent to the statement that the function $t \rightarrow \exp(-t)$ has the BMV-property.

Main Theorem. Every non-negative operator monotone decreasing function defined on the open positive half-line has the BMV-property.

3 Differential analysis

An simple proof of the following result can be found in [11, Proposition 1.3].

Proposition 3.1. The Fréchet differential of the exponential operator function $x \rightarrow \exp(x)$ is given by

$$d \exp(x)h = \int_{0}^{1} \exp(sx)h \exp((1-s)x) ds = \int_{0}^{1} A(s) \exp(x) ds$$

where $A(s) = \exp(sx)h \exp(-sx)$ for $s \in \mathbb{R}$. 

This is only a small part of the Dyson formula which contains formalisme developed earlier by Tomonaga, Schwinger and Feynman. The subject was given a rigorous mathematical treatment by Araki in terms of expansionals in Banach algebras. In particular [1, Theorem 3], the expansional

$$E_r(h; x) = \sum_{n=0}^{\infty} \int_0^1 \cdots \int_0^{s_{n-1}} A(s_n) A(s_{n-1}) \cdots A(s_1) ds_n ds_{n-1} \cdots ds_1$$

is absolutely convergent in the norm topology with limit

$$E_r(h; x) = \exp(x + h) \exp(-x).$$

We therefore obtain the pth Fréchet differential of the exponential operator function by the expression

$$d^p \exp(x) h^p$$

$$= p! \int_0^1 \cdots \int_0^{s_{p-1}} A(s_p) A(s_{p-1}) \cdots A(s_1) \exp(x) ds_p ds_{p-1} \cdots ds_1.$$

### 3.1 Divided differences

The following representation of divided differences is due to Hermite [12].

**Proposition 3.2.** Divided differences can be written in the following form

$$[x_0, x_1]_f = \int_0^1 f'(1-t_1)x_0 + t_1 x_1) dt$$

$$[x_0, x_1, x_2]_f = \int_0^1 \int_0^{t_1} f''(1-t_1)x_0 + (t_1 - t_2)x_1 + t_2 x_2) dt_2 dt_1$$

$$\vdots$$

$$[x_0, x_1, \ldots, x_n]_f = \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} f^{(n)}(1-t_1)x_0 + (t_1 - t_2)x_1 + \cdots + (t_{n-1} - t_n)x_{n-1} + t_n x_n) dt_n \cdots dt_2 dt_1$$

where $f$ is an n-times continuously differential function defined on an open interval $I$, and $x_0, x_1, \ldots, x_n$ are (not necessarily distinct) points in $I$.

### 3.2 Main technical tools

Taking the trace of the pth Fréchet differential of the exponential operator function [10, Theorem 3.4] one derive:
Theorem 3.3. Let $x$ and $h$ be operators on a Hilbert space of finite dimension $n$ written on the form

$$x = \sum_{i=1}^{n} \lambda_i e_{ii} \quad \text{and} \quad h = \sum_{i,j=1}^{n} h_{ij} e_{ij}$$

where $\{e_{ij}\}_{i,j=1}^{n}$ is a system of matrix units, and $\lambda_1, \ldots, \lambda_n$ and $h_{i,j}$ for $i, j = 1, \ldots, n$ are complex numbers. Then the $p$th derivative

$$\frac{d^p}{dt^p} \mathrm{Tr} \exp(x + th)\big|_{t=0} = p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} h_{i_1i_{p-1}} \cdots h_{i_{p-1}i_1} \lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_p}, \lambda_{i_1} \exp,$$

where $[\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_p}, \lambda_{i_1}]_{\exp}$ are divided differences of order $p+1$ of the exponential function.

Making use of the linearity of the function $f \rightarrow [x_0, x_1, \ldots, x_n]_f$ one obtains [10, Lemma 3.5 and Corollary 3.6] the following:

Corollary 3.4. Let $f : I \rightarrow \mathbb{R}$ be a $C^\infty$-function defined on an open and bounded interval $I$, and let $x$ and $h$ be self-adjoint operators on a Hilbert space of finite dimension $n$ written on the form

$$x = \sum_{i=1}^{n} \lambda_i e_{ii} \quad \text{and} \quad h = \sum_{i,j=1}^{n} h_{ij} e_{ij}$$

where $\{e_{ij}\}_{i,j=1}^{n}$ is a system of matrix units, and $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of $x$ counted with multiplicity. If the spectrum of $x$ is in $I$, then the trace function $t \rightarrow \mathrm{Tr} f(x + th)$ is infinitely differentiable in a neighborhood of zero and the $p$th derivative

$$\frac{d^p}{dt^p} \mathrm{Tr} f(x + th)\big|_{t=0} = p! \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} h_{i_1i_2} h_{i_2i_3} \cdots h_{i_{p-1}i_p} h_{i_p i_1} [\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_p}, \lambda_{i_1}]_f,$$

where $[\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_p}, \lambda_{i_1}]_f$ are divided differences of order $p+1$ of the function $f$. 
4 Proof of the main theorem

Proposition 4.1. Consider for a constant $c \geq 0$ the function

$$g(t) = \frac{1}{c + t} \quad t > 0.$$  

For arbitrary $n \times n$ matrices $x$ and $h$ such that $x$ is positive definite and $h$ is positive semi-definite we have

$$(-1)^p \frac{d^p}{dt^p} \operatorname{Tr} g(x + th) \bigg|_{t=0} \geq 0$$

for $p = 1, 2, \ldots$.  

Proof. Note that the divided differences of $g$ are of the form

$$(1) \quad [\lambda_1, \lambda_2, \ldots, \lambda_p]_g = (-1)^{p-1}g(\lambda_1)g(\lambda_2)\cdots g(\lambda_p) \quad p = 1, 2, \ldots.$$  

In the statement of Corollary 3.4 we set $\xi_i = g(\lambda_i)a_i$ and $b_i = g(\lambda_i)^{1/2}a_i$ where $a_i$ is the $i$th row in a matrix $a$ such that $h = aa^*$, and consequently $h_{ij} = (a_i | a_j)$. By calculation we then obtain:

$$\frac{(-1)^p}{p!} \frac{d^p}{dt^p} \operatorname{Tr} g(x + th) \bigg|_{t=0} = \sum_{i_1=1}^{n} \cdots \sum_{i_p=1}^{n} (\xi_{i_1} | b_{i_2})(b_{i_2} | b_{i_3})\cdots(b_{i_{p-1}} | b_{i_p})(b_{i_p} | \xi_{i_1}),$$

and it is not difficult to prove that such a sum is non-negative. QED

Proof of the main theorem. Consider again the function

$$g(t) = \frac{1}{c + t} \quad t > 0$$

for $c \geq 0$ and arbitrary $n \times n$ matrices $x$ and $h$ such that $x$ is positive definite and $h$ is positive semi-definite. We first note that

$$\frac{d^p}{dt^p} \operatorname{Tr} g(x + th) \bigg|_{t=0} = \frac{d^p}{dt^p} \operatorname{Tr} g(x + t_0h + \epsilon h) \bigg|_{\epsilon=0}$$

for $p = 1, 2, \ldots$ and $t_0 \geq 0$. The function $t \rightarrow \operatorname{Tr} g(x + th)$ is therefore completely monotone. Let now $f: \mathbb{R} \rightarrow \mathbb{R}$ be a non-negative operator monotone decreasing function. One may show [10] that $f$ allows the representation

$$f(t) = \beta + \int_{0}^{\infty} \frac{1}{c + t} d\nu(c)$$

for a positive measure $\nu$. The function $t \rightarrow \operatorname{Tr} f(x + th)$ is hence completely monotone and thus by Bernstein's theorem the Laplace transform of a positive measure with support in $[0, \infty)$. QED
4.1 Further analysis

One may try to use the Hermite expression in Proposition 3.2 to obtain a proof of the BMV-conjecture. Applying Theorem 3.3 and calculating the third derivative of the trace function we obtain

$$\frac{-1}{3!} \frac{d^3}{dt^3} \text{Tr} \exp(x - th) \bigg|_{t=0} = \sum_{p,i,j=1}^{n} (a_p | a_i)(a_i | a_j)(a_j | a_p)[\lambda_p \lambda_i \lambda_j \lambda_p]_{\exp}$$

$$= \int_{0}^{1} \int_{0}^{t_1} \int_{0}^{t_2} \sum_{p,i,j=1}^{n} (a_p | a_i)(a_i | a_j)(a_j | a_p) \exp((1-(t_1-t_3))\lambda_p + (t_1-t_2)\lambda_i + (t_2-t_3)\lambda_j) \, dt_3 \, dt_2 \, dt_1$$

where $h = aa^*$ and $a_i$ is the $i$th row in $a$. Assuming the BMV-conjecture this integral should be non-negative, and this would obviously be the case if the integrand is a non-negative function. However, there are examples [10, Example 4.2] where the integrand takes negative values.

Another way forward would be to examine the value of loops of the form

$$(a_1 | a_2)(a_2 | a_3) \cdots (a_{p-1} | a_p)(a_p | a_1)$$

since they, apart from an alternating sign, are the only possible negative factors in the expression of the derivatives of the trace functions. By applying a variational principle the lower bound

$$-\cos^p \left( \frac{\pi}{p} \right) \leq (a_1 | a_2)(a_2 | a_3) \cdots (a_{p-1} | a_p)(a_p | a_1)$$

was established in [9]. The lower bound converges very slowly to $-1$ as $p$ tends to infinity, and it is attained essentially only when all the vectors form a "fan" in a two-dimensional subspace.

Remark 4.2. If we only consider one-dimensional perturbations, that is if $h = cP$ for a constant $c > 0$ and a one-dimensional projection $P$, then $h$ is of the form $h = (\xi_i \xi_j)_{i,j=1, \ldots, n}$ for some vector $\xi = (\xi_1, \ldots, \xi_n)$ and each loop

$$h_{i_1 i_2} h_{i_2 i_3} \cdots h_{i_{p-1} i_p} h_{i_p i_1} = ||\xi_{i_1}||^2 \cdots ||\xi_{i_p}||^2$$

is manifestly real and non-negative. This implies that the trace function

$$t \to \text{Tr} \exp(-(x + th)),$$

for any self-adjoint $n \times n$ matrix $x$, is the Laplace transform of a positive measure with support in $[0, \infty)$. 
References


Frank Hansen: Institute of Economics, University of Copenhagen, Studiestraede 6, DK-1455 Copenhagen K, Denmark.