# A HYPER-GEOMETRIC APPROACH TO THE BMV-CONJECTURE

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ABSTRACT. We prove positivity of the BMV measure in dimension d = 3 in several non-trivial cases by combinatorial methods.

# 1. INTRODUCTION AND RESULTS

**Definition 1.** Let  $d \ge 1$  be fixed. Let A, B be complex, hermitian  $d \times d$  matrices and  $B \ge 0$ , then we denote

$$\phi^{A,B}(z) := \operatorname{tr}(\exp(A - zB))$$

for  $z \in \mathbb{C}$ .

The Bessis-Moussa-Villani conjecture (open since 1975, see [2]) asserts that the function  $\phi^{A,B}$  is completely monotone, i.e.,  $\phi^{A,B}$  is the Laplace transform of a **positive** measure  $\mu^{A,B}$  supported by  $[0,\infty[$ ,

$$\operatorname{tr}(\exp(A-zB)) = \int_0^\infty \exp(-zx)\mu^{A,B}(dx).$$

Since the function  $\phi^{A,B}$  is always Laplace transform of a possibly signed measure on  $[0,\infty[$ , we shall always denote this signed measure by  $\mu^{A,B}$ .

The BMV conjecture is closely related to convergence assertions on perturbation series in quantum mechanics and there is a substantial literature on it (recently [9] has been published, where several further references can be found, in particular we mention the review article [10]). We quote from [11]: "The BMV conjecture would

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entail a number of interesting inequalities not just for quantum partition functions, but also for their derivatives (a badly needed tool). Despite a lot of work, some by prominent mathematical physicists, only some simple cases have been decided. So far all results, including fairly extensive numerical experiments, are in agreement with the conjecture". As an example of recent progress on positive results we mention that the BMV-conjecture was shown to hold true in an average sense in [4]. Originally the BMV-conjecture was formulated more generally, namely, that  $z \mapsto \langle e, \exp(A - zB)e \rangle$  is completely monotone for each eigenvector e of B. This first conjecture was seen to be wrong immediately (see final part of [2]). In the appendix we provide a simple counter-example for the sake of completeness. For a deep equivalence to the validity of the BMV-conjecture see [9].

The remainder of this introductory section reviews some simple known facts on the BMV-conjecture.

**Proposition 1.** Let A, B be hermitian  $d \times d$  matrices,  $B \ge 0$ , then  $\phi^{A,B}(z) \ge 0$ for  $z \ge 0$  and

$$\frac{d}{dz}\phi^{A,B}(z) = -\operatorname{tr}(\exp(A - zB)B)$$
$$\frac{d^2}{dz^2}\phi^{A,B}(z) = \operatorname{tr}\left(\int_0^1 \exp(-s(A - zB))B\exp(s(A - zB))B\,ds\exp(A - zB)\right)$$
for  $z \ge 0$ . Hence  $-\frac{d}{dz}\phi^{A,B}(z) \ge 0$  and  $\frac{d^2}{dz^2}\phi^{A,B}(z) \ge 0$  for  $z \ge 0$ .

*Proof.* The first assertion follows from the fact that the eigenvalues of  $\exp(A - zB)$  are non-nenagtive and the second from the derivative of the function exp off 0 (see for instance [8], Theorem 38.2),

$$\frac{d}{dz}\exp(A-zB) = -\exp(A-zB)\int_0^1\exp(-s(A-zB))B\exp(s(A-zB))ds$$

Hence

$$\begin{aligned} \frac{d}{dz}\phi^{A,B}(z) &= -\operatorname{tr}\left(\exp(A-zB)\int_0^1 \exp(-s(A-zB))B\exp(s(A-zB))ds\right) \\ &= -\int_0^1 \operatorname{tr}\left(\exp(A-zB)\exp(-s(A-zB))B\exp(s(A-zB))\right)ds \\ &= -\int_0^1 \operatorname{tr}\left(\exp(A-zB)B\right)ds \\ &= -\operatorname{tr}(\exp(A-zB)B).\end{aligned}$$

The second formula follows by a similar reasoning. We conclude the inequalities in a "moving frame" associated to the eigenbasis of  $\exp[s(A - zB)]$ .

Bernstein's Theorem (see for instance [6]) asserts that a smooth function  $\phi$ :  $\mathbb{R}_{\geq 0} \to \mathbb{R}$  is the Laplace-transform of a non-negative measure  $\mu$  on  $\mathbb{R}_{\geq 0}$  if and only if  $(-1)^n \phi^{(n)}(z) \geq 0$  for  $z \geq 0$ . For the BMV-function  $\phi^{A,B}$  we know by the previous Lemma at least, that the Bernstein condition holds for n = 0, 1, 2. For dimension  $d \geq 3$  the case n = 3 is unknown in general. Having Bernstein's Theorem in mind, we see that the validity of the BMV-conjecture is equivalent to a sequence of interesting trace inequalities for hermitian matrices.

The following simple transformation properties are immediately proved.

- (1) Given a unitary matrix U in dimension d, then  $\mu^{UA\overline{U}^T, UB\overline{U}^T} = \mu^{A,B}$ . This is due to the unitary invariance of the trace functional.
- (2) Let  $I_d$  denote the identity matrix in dimension d. Then  $\mu^{A+\lambda_1 I_d,B} = \exp(\lambda_1)\mu^{A,B}$  for all real  $\lambda_1$ , since the identity matrix commutes with A, B.
- (3)  $\mu^{A,B+\lambda_2 I_d} = \mu^{A,B}(.+\lambda_2)$  for  $\lambda_2 \ge -b_{\min}$ , where  $b_{\min}$  denotes the minimal eigenvalue of B, since a translation of B by  $\lambda_2 I_d$  corresponds to a translation of the measure by  $\lambda_2$ .

Furthermore the following cases are known, where the BMV-conjecture holds true.

- (1) If A and B commute, the BMV-conjecture holds true.
- (2) If d = 1, 2, the BMV-conjecture holds true.
- (3) If B has at most two different eigenvalues, the BMV-conjecture holds true.
- (4) Let B be a diagonal matrix. If the off-diagonal elements of A are nonnegative, the Dyson expansion (see Section 2) yields that the BMV-conjecture holds true.

In view of all these well-known facts (for more investigations in these directions see [5]), the first non-trivial case, which appears in lowest non-trivial dimension, is the following. Take d = 3 and let without loss of generality  $B = diag(b_1, b_2, b_3)$  be a diagonal matrix and  $A = (a_{ij})$ , and assume  $a_{12}a_{13}a_{23} < 0$ . In this article we give – by hyper-geometric methods – a partial positive answer in this case.

We first analyse a representation of the measure  $\mu^{A,B}$  arising from the Dyson expansion. Our original approach was a stochastic one, but since we are able to draw our conclusion directly from the Dyson expansion, we leave away the stochastic reasonings (see the working paper [3]).

In Section 3 we concentrate on the 3-dimensional case, where we meet an important combinatorial simplification, which then leads to a summation problem in the theory of hyper-geometric series. Finally we are able to prove the following result.

**Theorem 1.** Given a real, symmetric  $3 \times 3$  matrix  $A = (a_{ij})$  and a diagonal matrix  $B = diag(b_1, b_2, b_3)$  with diagonal elements  $0 \le b_1 < b_3 < b_2$ . We assume that the following two conditions hold true:

- (1)  $\frac{|a_{12}|}{\sqrt{b_2-b_1}} \ge \frac{|a_{13}|}{\sqrt{b_3-b_1}}$  and  $\frac{|a_{12}|}{\sqrt{b_2-b_1}} \ge \frac{|a_{23}|}{\sqrt{b_2-b_3}}$ .
- (2)  $a_{11}(b_2 b_3) + a_{22}(b_3 b_1) + a_{33}(b_1 b_2) \ge 0.$

Then the function  $\phi^{A,B}(z) := \operatorname{tr}(\exp(A - zB))$  is completely monotone and the BMV-conjecture holds.

**Remark 1.** The unusual order  $b_1 < b_3 < b_2$  is due to the structure of our proof, see Section 3. Later we shall assume  $b_1 = 0$ , which is possible without restriction of generality as we have noted above under transformation property (3).

**Remark 2.** The two conditions in (1) are related to positivity of  $\mu^{A,B}$  on the intervals  $]0, b_3[$  and  $]b_3, b_2[$ , respectively (in this order). The second condition is a linear functional on the diagonal values of A.

**Remark 3.** The proof of Theorem 1 will be given in Section 5.

**Remark 4.** Furthermore the BMV-conjecture holds (trivially) if two of the three eigenvalues  $b_1, b_2, b_3$  agree or  $a_{12}a_{13}a_{23} \ge 0$ . Indeed, assume that  $a_{12}a_{13}a_{23} \ge 0$ , then we can make a change of coordinates such that  $a_{ij} \ge 0$  (for  $i \ne j$ ) by multiplying two coordinates by -1. If  $a_{ij} \ge 0$  holds for  $i \ne j$ , then by Theorem 2 the measure  $\mu^{A,B}$  is a sum of non-negative measures, hence non-negative. If  $b_2 = b_3$ , then B has a 2-dimensional eigenspace, where we can rotate without changing B, consequently we can find an orthogonal matrix U such that  $(U^TAU)_{23} = 0$  and  $U^TBU = B$ . The trace is invariant under rotations, so

$$\phi^{A,B}(z) = \operatorname{tr}(\exp(A - zB)) = \operatorname{tr}(\exp(U^T A U - z U^T B U)),$$

hence we find ourselves in the first trivial case.

#### 2. Representation of $\mu^{A,B}$

In this section we fix  $d \ge 2$  and a  $d \times d$  hermitian matrix A. We shall derive a series representation of the measure  $\mu^{A,B}$  applying Dyson's expansion (see for instance [10], p.624). We define a set  $C_n \subset \{1, \ldots, d\}^{n+1}$  of finite sequences  $(\gamma_1, \ldots, \gamma_{n+1})$ , which is characterized as set of all *n*-tuples such that no neighbors are equal, i.e.  $\gamma_i \neq \gamma_{i+1}$  for  $i = 1, \ldots, n$ , but  $\gamma_{n+1} = \gamma_1$ . Notice that  $C_0 = \{\{1\}, \ldots, \{d\}\}$  and  $C_1 = \emptyset$ . We denote  $C := \bigcup_{n \ge 0} C_n$ . Elements  $\gamma \in C_n$  are called **favorable paths** of length n. The map ord associates to  $\gamma \in C_n$  a monomial in the variables  $a_{ij}$ , which is called **order of the path**. The quantities  $l_{ij}(\gamma)$  are the respective powers of  $a_{ij}$  in the monomial  $\operatorname{ord}(\gamma)$ : for  $\gamma \in C_n$  we define

(2.1) 
$$\operatorname{ord}(\gamma) := a_{\gamma_1 \gamma_2} a_{\gamma_2 \gamma_3} \dots a_{\gamma_{n-1} \gamma_n} a_{\gamma_n \gamma_1}$$

(2.2) 
$$= \prod_{i < j} a_{ij}^{l_{ij}(\gamma)}.$$

The **characteristic** char $(\gamma) = (k_1(\gamma), \dots, k_d(\gamma))$  of a path  $\gamma \in C_n$  is defined by the number  $k_j(\gamma)$  of visits in state j (with at least one jump)

$$k_j(\gamma) := \#\{1 \le l \le n \text{ such that } \gamma_l = j\}.$$

Notice that the following formula holds for  $\gamma \in C_n$ ,

(2.3) 
$$\frac{1}{2}\sum_{j\neq i}l_{ij}(\gamma) = k_i(\gamma)$$

which leads in dimension 2 and 3 to one-to-one relations between  $char(\gamma)$  and  $ord(\gamma)$  (see Lemma 1).

We shall denote by  $\Delta_n$  the *n*-simplex in  $\mathbb{R}^{n+1}$ , i.e. the set of vectors  $(t_1, \ldots, t_{n+1}) \in \mathbb{R}^{n+1}$  with  $\sum_{i=1}^{n+1} t_i = 1$  and  $t_i \geq 0$ . On the *n*-simplex we shall consider the normalized uniform law  $\lambda_n$ , i.e.  $\lambda_n(\Delta_n) = 1$ . On the simplex  $\Delta_n$  with uniform law we define for a vector  $h \in \mathbb{R}^{n+1}$  the real-valued random variable  $\mathcal{Y}^h = \sum_{i=1}^{n+1} t_i h_i$ , and for  $g \in \mathbb{R}^{n+1}$  the measure  $Q^g$  with

$$\frac{dQ^g}{d\lambda_n} := \exp(\sum_{i=1}^{n+1} t_i g_i)$$

with respect to the uniform distribution  $\lambda_n$  on  $\Delta_n$ . The image measure of  $Q^g$  under  $\mathcal{Y}^h$  is denoted by  $\eta^{g;h}$ , which is a measure on  $\mathbb{R}$  with support in the convex hull of  $h_1, \ldots, h_{n+1}$ .

**Theorem 2.** Let A be a hermitian matrix, B a diagonal matrix with non-negative, mutually different entries  $b_1, \ldots, b_d$ . The diagonal elements of A are denoted by  $a_1, \ldots, a_d$ . Then the measure (see Definition 1)  $\mu^{A,B}$  is a signed measure decomposing into an absolutely continuous and singular part

(2.4) 
$$\mu^{A,B}(dx) = \sum_{i=1}^{d} \exp(a_i)\delta_{b_i}(dx) + \psi^{A,B}(x)dx.$$

The singular part corresponds to paths  $\gamma \in C$  with n = 0.  $\psi^{A,B}$  is a piecewise continuous function with possible discontinuities at  $b_i$  and with support in  $[\min_i b_i, \max_i b_i]$ . We have

(2.5) 
$$\psi^{A,B}(x) = \sum_{n \ge 2} \sum_{\gamma \in C_n} \phi(\gamma, x) \operatorname{ord}(\gamma),$$

where the density  $\phi(\gamma, x)$  is defined by

(2.6) 
$$\phi(\gamma, x) dx := \frac{1}{n!} \eta^{a_{\gamma_1}, \dots, a_{\gamma_n}, a_{\gamma_{n+1}}; b_{\gamma_1}, \dots, b_{\gamma_n}, b_{\gamma_{n+1}}} (dx)$$

for  $\gamma \in C_n$ .

*Proof.* By the calculation of ([10], p. 624) we obtain in our notation that

$$\operatorname{tr}(\exp(A-zB)) = \sum_{\gamma \in C} \frac{1}{n!} \int_{\Delta_n} \exp(-z\sum_{i=1}^{n+1} b_{\gamma_i} + a_{\gamma_i}) \lambda_n(dt_1, \dots, dt_{n+1}) \operatorname{ord}(\gamma)$$
$$= \sum_{\gamma \in C} \int_0^\infty \exp(-zx) \frac{1}{n!} \eta^{a_{\gamma_1}, \dots, a_{\gamma_n}, a_{\gamma_{n+1}}; b_{\gamma_1}, \dots, b_{\gamma_n}, b_{\gamma_{n+1}}}(dx) \operatorname{ord}(\gamma)$$
$$= \sum_{i=1}^d \exp(a_i) \delta_{b_i}(dx) + \psi^{A,B}(x) dx$$

holds true. Here it remains to show that the measure  $\eta^{a_{\gamma_1},...,a_{\gamma_n},a_{\gamma_{n+1}};b_{\gamma_1},...,b_{\gamma_n},b_{\gamma_{n+1}}}(dx)$ has a density. This can be seen from the fact that the intersection of  $\Delta_n$  and of the set  $\{\sum_{i=1}^{n+1} b_{\gamma_i} t_i = x\}$  depends in a differentiable way on x. The sum for  $\psi^{A,B}$ starts with n = 2, since there are no loops with only one jump.  $\Box$ 

**Example 1.** We illustrate the stochastic approach by the case d = 2. Since a loop  $\gamma \in C_n$  only appears if n is even and has the form 121... or 212..., the contributions in the above series are necessarily non-negative: indeed for a hermitian  $2 \times 2$  matrix A we must have that  $\operatorname{ord}(\gamma) \geq 0$  for all loops  $\gamma$  and the measures  $\eta$ 

are non-negative either. Hence the density is non-negative. Again we note that the validity of the BMV-conjecture for d = 2 is well-known (see e.g. [2]).

**Remark 5.** We have formulated Theorem 2 for Hermitian matrices A as this is presently our natural framework. We note that it may as well be formulated for general  $d \times d$  matrices A.

### 3. The case d = 3

From now on we assume d = 3 and w.l.g.  $b_1 = 0$ , we shall write  $a_i = a_{ii}$  for i = 1, 2, 3. In particular all matrices will be real from now on. We aim to calculate the measures  $\eta^{a_{\gamma_1},...,a_{\gamma_n},a_{\gamma_{n+1}};b_{\gamma_1},...,b_{\gamma_n},b_{\gamma_{n+1}}}$  for  $\gamma \in C$ ,  $n \geq 2$ .

We fix  $0 < b_3 \leq b_2$  and  $x \in ]0, b_3[$ . Due to the following choice of parameters we choose the unusual convention  $b_3 \leq b_2$ . The intersection of  $\Delta_2$  with the line  $\sum_{i=1}^{3} b_i \xi_i = x$  will be parametrized by

$$t \mapsto ((1 - x_2) + t(x_2 - x_3), x_2(1 - t), x_3t)$$

with real numbers  $0 < x_2 \le x_3 < 1$  and  $t \in [0, 1]$ . We shall denote this line segment by  $L^{x_2, x_3}$  and we obtain the relations

$$b_2 x_2 = x,$$
  
$$b_3 x_3 = x.$$

In particular we observe that – for given x – the numbers  $b_2, b_3$  and  $x_2, x_3$  determine each other. In order to obtain  $x_2 \leq x_3$  we have been choosing  $b_3 \leq b_2$ .

We apply the notions of the previous section. The **characteristic**  $\operatorname{char}(\gamma) = (k_1(\gamma), k_2(\gamma), k_3(\gamma))$  of a path  $\gamma \in C$  is the number of visits in the points 1, 2, 3 (where at least one jump appears, otherwise  $k_i(\gamma) = 0$ ). Clearly  $k_1 + k_2 + k_3 = n$ . We shall observe in the following Lemma that in dimension 3 the characteristic already determines the number of jumps between 1 - 2, 1 - 3 and 2 - 3, denoted by  $l_{12}, l_{13}$  and  $l_{23}$ . These quantities are defined via

$$a_{12}^{l_{12}(\gamma)}a_{13}^{l_{13}(\gamma)}a_{23}^{l_{23}(\gamma)} := a_{\gamma_1\gamma_2}a_{\gamma_2\gamma_3}\dots a_{\gamma_{n-1}\gamma_n}a_{\gamma_n\gamma_1} = \operatorname{ord}(\gamma)$$

and the numbers  $l_{ij}(\gamma)$  of jumps between *i* and *j* only depend on char  $(\gamma) = (k_1(\gamma), k_2(\gamma), k_3(\gamma))$  for  $\gamma \in C_n$ .

**Lemma 1.** The characteristic char $(\gamma) = (k_1(\gamma), k_2(\gamma), k_3(\gamma))$  of a path  $\gamma \in C$  and the powers  $(l_{12}(\gamma), l_{13}(\gamma), l_{23}(\gamma))$  of the order ord $(\gamma)$  are in one-to-one relation. By abuse of notation we may therefore write  $l_{ij}(\gamma) = l_{ij}(k_1(\gamma), k_2(\gamma), k_3(\gamma))$ .

*Proof.* We take formula (2.3) and solve it for  $l_{ij}$  given char( $\gamma$ ), we obtain

$$l_{12} = k_1 + k_2 - k_3$$
$$l_{13} = k_1 + k_3 - k_2$$
$$l_{23} = k_2 + k_3 - k_1$$

which yields the result.

Next we calculate in our particular setting (recall that d = 3 and  $b_1 = 0$ ) explicitly the density of  $\eta^{a_{\gamma_1},...,a_{\gamma_n},a_{\gamma_1};b_{\gamma_1},...,b_{\gamma_n},b_{\gamma_1}}$  at x.

**Lemma 2.** Define a probability density f on  $\Delta_2$  (with respect to uniform distribution  $\frac{1}{2}\lambda_2$  on  $\Delta_2$  of total mass  $\frac{1}{2}$ ) given through

(3.1) 
$$f(\xi_1,\xi_2,\xi_3) = \beta(k_1,k_2,k_3)\xi_1^{k_1-1}\xi_2^{k_2-1}\xi_3^{k_3-1}\exp(a_1\xi_1+a_2\xi_2+a_3\xi_3),$$

where

$$\beta(k_1, k_2, k_3) = \frac{(k_1 + k_2 + k_3 - 1)!}{(k_1 - 1)!(k_2 - 1)!(k_3 - 1)!}$$

for  $k_i \ge 1$ . We fix  $n \ge 2$ , a path  $\gamma \in C$  with characteristic char $(\gamma) = (k_1, k_2, k_3)$ ,  $n := k_1 + k_2 + k_3$ , and define

$$pr_{\gamma}: \Delta_n \to \Delta_2$$

through  $\xi_i(\gamma) := (pr_{\gamma}(t_1, \ldots, t_{n+1}))_i = \sum_{\substack{j=1\\\gamma_j=i}}^{n+1} t_j$  for i = 1, 2, 3. Then the following assertions hold true:

(1) Assume  $k_i \ge 1$ , for i = 1, 2, 3, then the law of the random variable  $pr_{\gamma}$  has density

(3.2) 
$$(k_1 + k_2 + k_3) \frac{\xi_{\gamma_1}}{k_{\gamma_1}} f(\xi_1, \xi_2, \xi_3) = n \frac{\xi_{\gamma_1}}{k_{\gamma_1}} f(\xi_1, \xi_2, \xi_3)$$

with respect to the measure  $\frac{1}{2}\lambda_2$  on  $\Delta_2$ . Notice that the state appearing in  $\gamma_1$  is counted twice in the density.

(2) For 
$$k_i \ge 1$$
,  $i = 1, 2, 3$ , and  $x \in ]0, b_3[$   
(3.3)  $\phi(\gamma, x) = \frac{1}{(n-1)!} \sqrt{\frac{1}{b_2 b_3}} \int_0^1 \left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \\ \frac{x_2(1-t)}{k_2} \\ \frac{x_3 t}{k_3} \end{array} \right\}$   
(3.4)  $f(1-x_2) + t(x_2-x_3), x_2(1-t), x_3 t) \sqrt{x_2 x_3} dt$ 

at  $0 < x < b_3$ , where the cases in {} pertain to  $\gamma_1 = 1, 2, 3$ . Notice the relations  $b_2x_2 = b_3x_3 = x$ .

- (3) Assume  $k_1 = 0$ , and  $x \in ]0, b_3[$ , then  $\phi(\gamma, x) = 0$  for all  $n \ge 2$ .
- (4) Assume  $k_2 = 0$ , and  $x \in ]0, b_3[$ , then

$$\phi(\gamma, x) = \frac{1}{(n-1)!} \frac{(k_1 + k_3 - 1)!}{(k_1 - 1)!(k_3 - 1)!} \exp\left[a_1(1 - x_3) + a_3x_3\right] \begin{cases} \frac{(1 - x_3)^{k_1} x_3^{k_3 - 1}}{k_1 b_3} & \text{if } \gamma_1 = 1\\ \frac{(1 - x_3)^{k_1 - 1} x_3^{k_3}}{k_3 b_3} & \text{if } \gamma_1 = 3 \end{cases}$$

and  $n \geq 2$  is necessarily even.

(5) Assume  $k_3 = 0$ , and  $x \in ]0, b_3[$ , then

$$\phi(\gamma, x) = \frac{1}{(n-1)!} \frac{(k_1 + k_2 - 1)!}{(k_1 - 1)!(k_2 - 1)!} \exp\left[a_1(1 - x_2) + a_2 x_2\right] \begin{cases} \frac{(1 - x_2)^{k_1} x_2^{k_2 - 1}}{k_1 b_2} & \text{if } \gamma_1 = 1\\ \frac{(1 - x_2)^{k_2 - 1} x_2^{k_2}}{k_2 b_2} & \text{if } \gamma_1 = 2 \end{cases}$$

and  $n \geq 2$  is necessarily even.

Proof. Fix ,  $n \geq 2$  and  $k_i \geq 1$  for i = 1, 2, 3. Fix furthermore  $\gamma \in C_n$  and let  $(\gamma_1, \ldots, \gamma_n, \gamma_{n+1}) \in C_n$ . We first set  $a_i = 0$  for i = 1, 2, 3. By direct computation we verify that now f indeed defines a probability measure on  $\Delta_2$ , hence the norming factor is correct (the actual form of f stems from pushing forward with  $pr_{\gamma}$  and simply observing that a sum of independent uniformly distributed variables in the simplex leads to a  $\beta$ -distribution). In the chart  $\pi_{12}$  (projection from  $\Delta_2$  on the first two components in  $\mathbb{R}^3$ ) the volume element  $\frac{1}{2}\lambda_2(d\xi)$  equals  $d\xi_1 d\xi_2$  on  $\{(\xi_1, \xi_2) \in \mathbb{R}^2, \xi_1, \xi_2 \geq 0, \xi_1 + \xi_2 \leq 1\}$ .

$$\begin{aligned} \frac{1}{2} \int_{\Delta_2} f(\xi_1, \xi_2, \xi_3) \lambda_2(d\xi) &= \beta(k_1, k_2, k_3) \int_0^1 \int_0^{1-\xi_2} \xi_1^{k_1-1} \xi_2^{k_2-1} (1-\xi_1-\xi_2)^{k_3-1} d\xi_1 d\xi_2 \\ &= \beta(k_1, k_2, k_3) \int_0^1 \xi_2^{k_2-1} (1-\xi_2)^{k_1+k_3-1} \int_0^{1-\xi_2} \frac{\xi_1^{k_1-1}}{(1-\xi_2)^{k_1-1}} (1-\frac{\xi_1}{1-\xi_2})^{k_3-1} d(\frac{\xi_1}{1-\xi_2}) d\xi_2 \\ &= \beta(k_1, k_2, k_3) \int_0^1 \xi_2^{k_2-1} (1-\xi_2)^{k_1+k_3-1} \int_0^1 \eta^{k_1-1} (1-\eta)^{k_3-1} d\eta d\xi_2 \\ &= \beta(k_1, k_2, k_3) \frac{(k_2-1)!(k_1+k_3-1)!}{(k_1+k_2+k_3-1)!} \frac{(k_1-1)!(k_3-1)!}{(k_1+k_3-1)!} = 1. \end{aligned}$$

We continue now with general  $a_i$ . Calculating the formula of the density  $\phi(\gamma, x)$  at  $x \in ]0, b_3[$  amounts to calculating the mass of  $pr_{\gamma}$  passed by the line  $L^{x_2, x_3}$  through variations in x. Fixing  $b_2, b_3$  we thus fix  $x_2, x_3$ . The area of the quadrangle with corners at  $e_1 + x_i(e_i - e_1)$ ,  $e_1 + (x_i + dx_i)(e_i - e_1)$ , for i = 2, 3, with respect to the measure  $\frac{1}{2}\lambda_2(d\xi)$  – under a small variation dx of x – is given by

$$\frac{1}{2}(x_3dx_2 + x_2dx_3) = \frac{1}{b_3b_2}xdx$$
$$= \frac{1}{b_3b_2}\sqrt{b_2b_3x_2x_3}dx$$
$$= \sqrt{\frac{1}{b_2b_3}}\sqrt{x_2x_3}dx.$$

Shrinking the side conv $\{e_1 + x_2(e_2 - e_1), e_1 + x_3(e_3 - e_1)\}$  to an infinitesimal element at the point  $((1 - x_2) + t(x_2 - x_3), x_2(1 - t), x_3t)$ , for  $t \in [0, 1]$ , on  $L^{x_2, x_3}$  leads to the appropriate area element

$$\sqrt{\frac{1}{b_2 b_3}} \sqrt{x_2 x_3} dx dt.$$

Hence we can determine  $\phi_n(\gamma, x)$  through equation (2.6) and formula (3.2) evaluated at  $((1 - x_2) + t(x_2 - x_3), x_2(1 - t), x_3t)$ , for  $t \in [0, 1]$ ,

$$P_{\gamma}(b_{2}\xi_{2} \circ p_{n} + b_{3}\xi_{3} \circ p_{n} \in [x, x + dx])$$

$$= \sqrt{\frac{1}{b_{2}b_{3}}}\sqrt{x_{2}x_{3}}dx \frac{1}{(n-1)!}\beta(k_{1}, k_{2}, k_{3}) \int_{0}^{1} \left\{ \begin{array}{c} \frac{(1-x_{2})+t(x_{2}-x_{3})}{k_{1}} \\ \frac{x_{2}(1-t)}{k_{2}} \\ \frac{x_{3}t}{k_{3}} \end{array} \right\}$$

$$f(1-x_{2}+t(x_{2}-x_{3}), x_{2}(1-t), x_{3}t)dt.$$

For the degenerate cases  $(n \ge 2, k_2 = 0 \text{ or } k_3 = 0)$ , we perform the same program. We first calculate the density of the law of  $pr_{\gamma}$  if one of the  $k_i$  is zero, which is a density supported by one edge of the simplex  $\Delta_2$ . Assume  $k_3 = 0$ . With respect to the uniform distribution with total mass 1 on the edge conv $\{e_1, e_2\}$  of  $\Delta_2$  we obtain for  $k_1, k_2 \ge 1$ 

$$(k_1 + k_2)\frac{\xi_{\gamma_1}}{k_{\gamma_1}}\frac{(k_1 + k_2 - 1)!}{(k_1 - 1)!(k_2 - 1)!}\xi_1^{k_1 - 1}\xi_2^{k_2 - 1}\exp(a_1\xi_1 + a_2\xi_2)$$

and similar for the other case. A small variation dx in x leads via  $\frac{dx}{b_i} = dx_i$  for i = 2, 3 to the desired results.

In order to write the above densities in a more compact way we shall apply the well-known formula

$$\frac{1}{\Gamma(\alpha)} \int_0^1 g(t) t^{\alpha - 1} \to g(0)$$

as  $\alpha \downarrow 0$  for any continuous function  $g : [0,1] \to \mathbb{R}$ . Hence we can apply  $(k-1)! = \Gamma(k)$  for  $k \ge 0$  and obtain the following proposition:

**Lemma 3.** For  $\gamma \in C_n$ ,  $n \geq 2$  and  $x \in ]0, b_3[$ , we obtain in the sense of Gammafunctions

$$\phi(\gamma, x) = \frac{1}{(n-1)!} \sqrt{\frac{1}{b_2 b_3}} \int_0^1 \left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \\ \frac{x_2(1-t)}{k_2} \\ \frac{x_3 t}{k_3} \end{array} \right\}$$
$$f(1-x_2+t(x_2-x_3), x_2(1-t), x_3 t) \sqrt{x_2 x_3} dt$$

for char( $\gamma$ ) =  $(k_1, k_2, k_3)$ ,  $k_1 + k_2 + k_3 = n$ , and  $k_i \ge 0$ , where the cases in {} pertain to  $\gamma_1 = 1, 2, 3$ .

*Proof.* For  $k_i \ge 1$  there is nothing to prove. Assume now that we take the limit  $k_2 \downarrow 0$ , hence  $\gamma_2 = 1$  or 3, since the vertex 2 cannot be starting point. We introduce furthermore

$$\lambda := a_1(x_2 - x_3) - a_2x_2 + a_3x_3$$
$$\mu := a_1(1 - x_2) + a_2x_2$$

as in Remark 6. Hence the limit yields

$$\begin{split} \lim_{\alpha \downarrow 0} \frac{1}{(n-1)!} \frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!} \sqrt{\frac{1}{b_2 b_3}} \frac{1}{\Gamma(\alpha)} \int_0^1 \left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \text{ if } \gamma_1 = 1\\ \frac{x_3 t}{k_3} \text{ if } \gamma_1 = 3 \end{array} \right\} \\ & ((1-x_2)+t(x_2-x_3))^{k_1-1} (x_2(1-t))^{\alpha-1} (x_3 t)^{k_3-1} \sqrt{x_2 x_3} dt\\ & = \frac{\exp(\lambda+\mu)}{(n-1)!} \frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!} \frac{1}{x_2} \sqrt{\frac{x_2 x_3}{b_2 b_3}} \left\{ \begin{array}{c} \frac{(1-x_3)^{k_1} x_3^{k_3-1}}{k_1} \text{ if } \gamma_1 = 1\\ \frac{(1-x_3)^{k_1-1} x_3^{k_3}}{k_3} \text{ if } \gamma_1 = 3 \end{array} \right\} \\ & = \frac{\exp(\lambda+\mu)}{(n-1)!} \frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!} \left\{ \begin{array}{c} \frac{(1-x_3)^{k_1} x_3^{k_3-1}}{k_1 b_3} \text{ if } \gamma_1 = 1\\ \frac{(1-x_3)^{k_1-1} x_3^{k_3}}{k_3 b_3} \text{ if } \gamma_1 = 3 \end{array} \right\} \end{split}$$

since  $x_2b_2 = x_3b_3 = x$ . Similarly for the third case.

For the calculation of the BMV-measure  $\mu^{A,B}$  we can make an essential further simplification: it turns out that if we average over all paths  $\gamma$  with fixed characteristic char( $\gamma$ ) (and varying the first entry  $\gamma_1$ ) formulas (3.3)-(3.6) appear in a simpler

form, which only depends on the characteristic. For  $n \ge 2$  we define the density

$$\chi(k_1, k_2, k_3, x) := \frac{1}{\#\{\gamma \in C : \text{ char}(\gamma) = (k_1, k_2, k_3)\}} \sum_{\substack{\gamma \in C \\ \text{char}(\gamma) = (k_1, k_2, k_3)}} \phi(\gamma, x),$$

i.e. the average of the densities  $\phi(\gamma, x)$  where  $\gamma$  ranges through the paths with fixed characteristic  $(k_1, k_2, k_3)$ .

**Lemma 4.** We fix a path  $\gamma \in C$  with characteristic char $(\gamma) = (k_1, k_2, k_3)$  for  $n \geq 2$ . Then the following assertion holds,

(3.7) 
$$\chi(k_1, k_2, k_3, x) = \sqrt{\frac{1}{b_2 b_3}} \frac{1}{n!} \int_0^1 f(1 - x_2 + t(x_2 - x_3), x_2(1 - t), x_3 t) \sqrt{x_2 x_3} dt$$

in the sense of Gamma-functions.

**Remark 6.** The exponential term in (3.1) simplifies to  $e^{\lambda t+\mu}$  with  $\lambda = a_1(x_2 - x_3) - a_2x_2 + a_3x_3$  and  $\mu = a_1(1 - x_2) + a_2x_2$ . Hence we obtain, for a path with characteristic char $(\gamma) = (k_1, k_2, k_3)$ ,  $n \ge 2$ , by the binomial theorem and the Beta integral that

$$\chi(k_1, k_2, k_3, x) = \frac{(1 - x_2)^{k_1 - 1} x_2^{k_2} x_3^{k_3}}{nx}$$
$$\times \sum_{L \ge 0} \sum_{r=0}^{k_1 - 1} e^{\mu} \frac{\lambda^L}{L!} {\binom{k_1 - 1}{r}} \left(\frac{x_2 - x_3}{1 - x_2}\right)^r \frac{(k_3)_{L+r}}{(k_1 - 1)!(k_2 + k_3 + L + r - 1)!},$$

holds true, or — by using t = 1 - s — an alternate representation,

$$\chi(k_1, k_2, k_3, x) = \frac{(1 - x_3)^{k_1 - 1} x_2^{k_2} x_3^{k_3}}{nx}$$
$$\times \sum_{L \ge 0} \sum_{r=0}^{k_1 - 1} {\binom{k_1 - 1}{r}} e^{\mu + \lambda} \frac{(-\lambda)^L}{L!} \left(\frac{x_3 - x_2}{1 - x_3}\right)^r \frac{(k_2)_{L+r}}{(k_1 - 1)!(k_2 + k_3 + L + r - 1)!}$$

Here we apply the notation  $(k)_r := \frac{\Gamma(r+k)}{\Gamma(k)}$ .

Proof of Lemma 4. Fix  $n \ge 2$ . For the proof we apply the representations of the densities (3.3)-(3.6), and the fact that among all paths  $\gamma \in C_n$  with characteristic char $(\gamma) = (k_1, k_2, k_3)$  the path with  $\gamma_1 = i$  appear with relative frequency  $\frac{k_i}{n}$ , hence absolutely

$$\#\{\gamma \in C: \quad \operatorname{char}(\gamma) = (k_1, k_2, k_3)\}\frac{k_i}{n}$$

times. We calculate the density  $\chi(k_1, k_2, k_3, x)$  at  $x \in ]0, b_3[$ . This leads for  $k_i \ge 1$  $\operatorname{to}$ 

$$\begin{split} \chi(k_1, k_2, k_3, x) &= \frac{1}{\#\{\gamma \in C : \operatorname{char}(\gamma) = (k_1, k_2, k_3)\}} \sum_{\substack{\gamma \in C \\ \operatorname{char}(\gamma) = (k_1, k_2, k_3)}} \phi(\gamma, x) \\ &= \frac{1}{(n-1)!} \sqrt{\frac{1}{b_2 b_3}} \int_0^1 \left(\frac{k_1}{n} \frac{(1-x_2) + t(x_2 - x_3)}{k_1} + \frac{k_2}{n} \frac{x_2(1-t)}{k_2} + \frac{k_3}{n} \frac{x_3 t}{k_3}\right) \\ &= \frac{1}{n!} \sqrt{\frac{1}{b_2 b_3}} \int_0^1 f(1-x_2 + t(x_2 - x_3), x_2(1-t), x_3 t) \sqrt{x_2 x_3} dt \\ &= \frac{1}{n!} \sqrt{\frac{1}{b_2 b_3}} \int_0^1 f(1-x_2 + t(x_2 - x_3), x_2(1-t), x_3 t) \sqrt{x_2 x_3} dt. \end{split}$$

For  $k_1 = 0$  we conclude directly, since the density vanishes. For  $k_2 = 0$  we use

$$\chi(k_1, 0, k_3, x) = \frac{1}{(n-1)!} \frac{k_1}{n} \frac{(k_1 + k_3 - 1)!}{k_1!(k_3 - 1)!} \frac{x_3^{k_3 - 1}(1 - x_3)^{k_1}}{b_3} \exp(a_1(1 - x_3) + a_3x_3) + \frac{1}{(n-1)!} \frac{k_3}{n} \frac{(k_1 + k_3 - 1)!}{(k_1 - 1)!k_3!} \frac{x_3^{k_3}(1 - x_3)^{k_1 - 1}}{b_3} \exp(a_1(1 - x_3) + a_3x_3) = \frac{1}{n!} \frac{(k_1 + k_3 - 1)!}{(k_1 - 1)!(k_3 - 1)!} \frac{x_3^{k_3 - 1}(1 - x_3)^{k_1 - 1}}{b_3} \exp(a_1(1 - x_3) + a_3x_3)$$
and analogously for  $k_3 = 0$ .

and analogously for  $k_3 = 0$ .

For the case  $x \in ]b_3, b_2[$  we shall apply the following parametrization

$$t \mapsto ((1-t)y_1, (1-y_1) + t(y_1 - y_3), ty_3)$$

for  $0 \le y_1 \le y_3 \le 1$  satisfying the relations

$$b_2 y_1 = b_2 - x$$
  
 $b_2 - b_3 y_3 = b_2 - x.$ 

This leads as in the proof of Lemma 5 to the volume element

(

$$\frac{1}{\sqrt{b_2(b_2-b_3)}}\sqrt{y_1y_3}dx$$

under variations of x, hence the respective densities  $\chi$  satisfy the following relations: we fix a path  $\gamma \in C_n$  with characteristic char $(\gamma) = (k_1, k_2, k_3), k_1 + k_2 + k_3 = n$  for  $n \geq 2$ , hence

(3.8)

$$\chi(k_1, k_2, k_3, x) = \sqrt{\frac{1}{b_2(b_2 - b_3)}} \frac{1}{n!} \int_0^1 f((1 - t)y_1, 1 - y_1 + t(y_1 - y_3), ty_3) \sqrt{y_1 y_3} dt$$

in the sense of Gamma-functions.

**Remark 7.** Notice that the case  $x \in ]b_3, b_2[$  is deduced from the case  $x \in ]0, b_2[$ when the permutation  $1 \leftrightarrow 2$  is performed. One replaces then  $x_2$  by  $y_1, x_3$  by  $y_3$ , performs the permutation for  $a_{ij}$ , and replaces  $b_2$  by  $b_2$  and  $b_3$  by  $b_2 - b_3$ . All the necessary relations maintain and the first case in full generality then implies the second one.

#### 4. Combinatorial Sums

Our next goal is to represent  $\psi^{A,B}(x) := \psi(x)$  in the following way. By Remark 7 it suffices to consider the interval  $]0, b_3[$ .

**Proposition 2.** Suppose that  $b_2 > b_3$ . Then, for  $x \in ]0, b_3[$ , we have

$$\begin{split} \psi(x) &= \sum_{\gamma \in C} \chi(k_1, k_2, k_3, x) \operatorname{ord}(\gamma) \\ &= \frac{1}{x} \sum_{k \ge 1} \sum_{m \ge 0} \sum_{l \ge 0, l \equiv m \mod 2} (1 - x_3)^{k-1} e^{\lambda + \mu} \sum_{L \ge 0} \frac{(-\lambda)^L}{L!} \\ &\times \sum_{r=0}^{k-1} \binom{k-1}{r} \left(\frac{x_3 - x_2}{1 - x_3}\right)^r \frac{\left(\frac{2k + m - l}{2}\right)_{r+L}}{k! (k + m + r + L - 1)!} \\ &\times \sum_{0 \le j \le k, j \equiv m \mod 2} \binom{k}{j} \binom{\frac{m-j}{2} + k - 1}{k - 1} \binom{k-j}{\frac{l-j}{2}} 2^j \\ &\times (a_{12}\sqrt{x_2})^{2k-l} (a_{13}\sqrt{x_3})^l (a_{23}\sqrt{x_2x_3})^m \end{split}$$

The *proof* of Proposition 2 is just a direct combination of Remark 6, the following Lemma 5 and the representations  $l_{12} = 2k-l$ ,  $k_2 = (2k-l+m)/2$ , and  $k_3 = (l+m)/2$ when  $k_1 = k$ ,  $l_{13} = l$ , and  $l_{23} = m$  are given.

However, the representation of  $\psi(x)$  in Proposition 2 has to be transformed in a proper way to observe that it is non-negative. For this purpose we will further introduce the hypergeometric function F(a, b; c; z) and use certain hypergeometric identities in order to simplify the above representation.

#### 4.1. Counting paths on the triangle.

**Lemma 5.** The number of paths  $\gamma$  in C with  $k_1(\gamma) = k$ ,  $l_{13}(\gamma) = l$ ,  $l_{23}(\gamma) = m$ and  $l \equiv m \mod 2$  is given through

(4.1) 
$$\frac{2k+m}{k} \sum_{0 \le j \le k, j \equiv m \mod 2} \binom{k}{j} \binom{\frac{m-j}{2}+k-1}{k-1} \binom{k-j}{\frac{l-j}{2}} 2^j.$$

If  $l \not\equiv m \mod 2$ , then the number of paths vanishes (if n = 0, one has to "interpret"  $\frac{2k+m}{k}$  as 3).

*Proof.* From [7] we get that the generating function of  $\operatorname{ord}(\gamma)$  of all paths  $\gamma$  with  $\gamma_1 = 1$  is given by

$$\sum_{\gamma,\gamma_1=1} \operatorname{ord}(\gamma) = \frac{\begin{vmatrix} 1 & -a_{23} \\ -a_{23} & 1 \end{vmatrix}}{\begin{vmatrix} 1 & -a_{12} & -a_{13} \\ -a_{12} & 1 & -a_{23} \\ -a_{13} & -a_{23} & 1 \end{vmatrix}}$$
$$= \frac{1 - a_{23}}{1 - 2a_{12}a_{13}a_{23} - a_{12}^2 - a_{13}^2 - a_{23}^2}.$$

Hence, if  $P_1(k, l, m)$  denotes the number of paths  $\gamma$  in C with  $k_1(\gamma) = k$ ,  $l_{13}(\gamma) = l$ ,  $l_{23}(\gamma) = m$ , and  $\gamma_1 = 1$  we have

$$\sum_{k,l,m} P_1(k,l,m) x^k a_{13}^l a_{23}^m = \frac{1 - a_{23}^2}{1 - a_{23}^2 - x(2a_{13}a_{23} + a_{13}^2 + 1)}.$$

From that we immediately get (if  $l \equiv m \mod 2$ )

$$P_1(k, l, m) = \sum_{0 \le j \le k, j \equiv m \mod 2} {\binom{k}{j} \binom{\frac{m-j}{2} + k - 1}{k - 1} \binom{k-j}{\frac{l-j}{2}} 2^j}.$$

Finally, if we denote by P(k, l, m) the total number of paths  $\gamma$  in C with  $k_1(\gamma) = k$ ,  $l_{13}(\gamma) = l$ , and  $l_{23}(\gamma) = m$  then

$$\frac{1}{k}P_1(k,l,m) = \frac{1}{n}P(k,l,m),$$

where  $n = 2k + m = k_1 + k_2 + k_2$ . This proves (4.1).

4.2. Hypergeometric identities. The hypergeometric function F(a, b; c; z) is defined (for complex |z| < 1) by

$$F(a,b;c;z) = \sum_{n\geq 0} \frac{(a)_n(b)_n}{(c)_n n!} z^n,$$

where  $(x)_n = \Gamma(x+n)/\Gamma(x) = x(x+1)\cdots(x+n-1)$  denote the rising factorials. There are lots of identities (see [1, Chapter 15]) for these kinds of functions. Some of them will be used in the sequel. For example one has Euler's integral representation

$$F(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 (1-zt)^{-a} t^{b-1} (1-t)^{c-b-1} dt$$

if |z| < 1 and  $\Re(c) > \Re(b) > 0$ . Furthermore, it was already known to Gauss that

(4.2) 
$$F(a,b;c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}$$

if  $\Re(c - a - b) > 0$ .

We start with a lemma, where we use the identity

(4.3) 
$$F(a,b;c;z) = (1-z)^{-a}F\left(a,c-b;c,\frac{z}{z-1}\right).$$

**Lemma 6.** Suppose that  $j \equiv m \mod 2$ . Then

$$2^{j} \sum_{l \ge j, l \equiv j \mod 2} {\binom{k-j}{\frac{l-j}{2}} \left(\frac{2k+m-l}{2}\right)_{r} C^{l} D^{2k-l}} = (C^{2} + D^{2})^{k} v^{j} \sum_{\rho=0}^{r} (-1)^{\rho} {\binom{r}{\rho}} \left(\frac{2k+m-j}{2}\right)_{r-\rho} \frac{(k-j)!}{(k-j-\rho)!} \left(\frac{C}{2D}v\right)^{\rho},$$

where  $v = 2CD/(C^2 + D^2)$ .

Proof. We note that the left hand side of the above equation can be represented as

$$2^{j}(CD)^{j}d^{2(k-j)}\left(\frac{2k+m-j}{2}\right)_{r} \times F\left(-(k-j), -\left(\frac{2k+m-j}{2}-1\right); -\left(\frac{2k+m-j}{2}+r-1\right); -\frac{C^{2}}{D^{2}}\right)$$

and the right hand side as

$$(C^{2} + D^{2})^{k-j} (2CD)^{j} \left(\frac{2k+m-j}{2}\right)_{r} \times F\left(-(k-j), -r; -\left(\frac{2k+m-j}{2}+r-1\right); \frac{C^{2}}{C^{2}+D^{2}}\right).$$

By using (4.3) with

$$a = -(k-j), \ b = -\left(\frac{2k+m-j}{2}-1\right), \ c = -\left(\frac{2k+m-j}{2}+r-1\right)$$

and  $z = -C^2/D^2$  we directly get a proof of the lemma.

4.3. Further Hypergeometric Identities. In this section we present a proof of rather strange identities that seem to be new in the context of hypergeometric series.

We set

$$A_r(k;v,\xi) := \sum_{m \ge 0} \sum_{j=0}^k \binom{k}{j} \frac{2^{k+r-1} \left(\frac{m-j+2}{2}\right)_{k+r-1}}{(m+1)_{k+2r-1}} v^j \frac{\xi^m}{m!},$$

where r a is non-negative integer.

# Lemma 7. We have

$$\begin{split} A_0(k;v,\xi) &= (1+v)^k e^{\xi} \\ &+ \int_0^1 \sum_{\ell \ge 0} \frac{k!}{\ell!(\ell+1)!(k-2\ell-2)!} (1+sv)^{k-2\ell-2} \left(\frac{1-v^2}{2}\right)^{\ell+1} \left(\frac{1-s^2}{2}\right)^{\ell} e^{s\xi} \, ds \\ &= (1+v)^k e^{\xi} \\ &+ \binom{k}{2} (1-v^2) \int_0^1 (1+sv)^{k-2} F\left(-\frac{k-2}{2}, -\frac{k-3}{2}; 2; \frac{(1-v^2)(1-s^2)}{(1+sv)^2}\right) e^{s\xi} \, ds \end{split}$$

and

$$\begin{split} &A_r(k;v,\xi) \\ &= \int_0^1 \sum_{\ell \ge 0} \frac{k!}{\ell!(\ell+r-1)!(k-2\ell)!} (1+sv)^{k-2\ell} \left(\frac{1-v^2}{2}\right)^\ell \left(\frac{1-s^2}{2}\right)^{\ell+r-1} e^{s\xi} \, ds \\ &= \int_0^1 \frac{(1+sv)^k}{(r-1)!} \left(\frac{1-s^2}{2}\right)^{r-1} F\left(-\frac{k}{2}, -\frac{k-1}{2}; r; \frac{(1-v^2)(1-s^2)}{(1+sv)^2}\right) e^{s\xi} \, ds, \end{split}$$

where r a is positive integer.

**Remark 8.** Note that the right hand sides of these identities are non-negative if  $|v| \leq 1$ . Hence, we have  $A_r(k; v, \xi) \geq 0$ .

In fact, we are more interested in sums of the form

$$\tilde{A}_{r}(k;v,\xi) = \frac{1}{2} \left( A_{r}(k;v,\xi) + A_{r}(k;-v,-\xi) \right)$$
$$= \sum_{m \ge 0} \sum_{0 \le j \le k, \ j \equiv m \bmod 2} \binom{k}{j} \frac{2^{k+r-1} \left(\frac{m-j+2}{2}\right)_{k+r-1}}{(m+1)_{k+2r-1}} v^{j} \frac{\xi^{m}}{m!}.$$

Since  $A_r(k; v, \xi) \ge 0$  and  $A_r(k; -v, -\xi) \ge 0$  (for  $|v| \le 1$ ) we also have  $\tilde{A}_r(k; v, \xi) \ge 0$ and the representations

$$\begin{split} \tilde{A}_0(k;v,\xi) &= \frac{(1+v)^k}{2} e^{\xi} + \frac{(1-v)^k}{2} e^{-\xi} \\ &+ \binom{k}{2} \frac{1-v^2}{2} \int_{-1}^1 (1+sv)^{k-2} F\left(-\frac{k-2}{2}, -\frac{k-3}{2}; 2; \frac{(1-v^2)(1-s^2)}{(1+sv)^2}\right) e^{s\xi} \, ds \end{split}$$

and

$$\begin{split} \tilde{A}_r(k;v,\xi) \\ &= \frac{1}{2} \int_{-1}^1 \frac{(1+sv)^k}{(r-1)!} \left(\frac{1-s^2}{2}\right)^{r-1} F\left(-\frac{k}{2}, -\frac{k-1}{2}; r; \frac{(1-v^2)(1-s^2)}{(1+sv)^2}\right) e^{s\xi} \, ds, \end{split}$$

where r a is positive integer.

*Proof.* <sup>1</sup> We prove first the case of positive r. Both sides of the identity are power series in v and  $\xi$ . Thus, it is sufficient to compare coefficients. The coefficient of  $v^j \xi^m/m!$  of the right hand side is given by

By applying the substitution  $s = \sqrt{t}$ , integrating the corresponding Beta integrals and rewriting the sum over  $\ell$  in hypergeometric notation we thus get

$$\begin{split} &\int_{0}^{1} \sum_{\ell \geq 0} \frac{k!}{\ell! (\ell + r - 1)! (k - 2\ell)!} \\ &\quad \times \sum_{i \geq 0} (-1)^{i} \binom{\ell}{i} \frac{1}{2^{2i+r}} \binom{k - 2\ell}{j - 2i} t^{m/2 + j/2 - i - 1/2} (1 - t)^{\ell + r - 1} dt \\ &= \sum_{\ell \geq 0} \frac{k!}{\ell! (\ell + r - 1)! (k - 2\ell)!} \\ &\quad \times \sum_{i \geq 0} (-1)^{i} \binom{\ell}{i} \frac{1}{2^{2i+r}} \binom{k - 2\ell}{j - 2i} \frac{\Gamma(m/2 + j/2 - i + 1/2)\Gamma(\ell + r)}{\Gamma(\ell + r + m/2 + j/2 - i + 1/2)} \\ &= \sum_{i \geq 0} \frac{(-1)^{i} (1 + i)_{k - i}}{2^{2i+r} (j - 2i)! (k - j)! (\frac{1}{2} + i + \frac{j}{2} + \frac{m}{2})_{i + r}} \\ &\quad \times F\left(\frac{j}{2} - \frac{k}{2}, \frac{1}{2} + \frac{j}{2} - \frac{k}{2}; \frac{1}{2} + \frac{j}{2} + \frac{m}{2} + r; 1\right). \end{split}$$

Next we use formula (4.2) and obtain (after rewriting the remaining sum in hypergeometric notation)

$$\binom{k}{j} \frac{\Gamma\left(\frac{1}{2} + \frac{j}{2} + \frac{m}{2}\right) \Gamma\left(-\frac{j}{2} + k + \frac{m}{2} + r\right)}{2^{r} \Gamma\left(\frac{k}{2} + \frac{m}{2} + r\right) \Gamma\left(\frac{1}{2} + \frac{k}{2} + \frac{m}{2} + r\right)} F\left(-\frac{j}{2}, \frac{1}{2} - \frac{j}{2}; \frac{1}{2} - \frac{j}{2} - \frac{m}{2}; 1\right).$$

In order to avoid difficulties with zero-cancellations we interpret this sum as a limit, use again formula (4.2) and obtain (after some algebra)

$$\begin{split} &\lim_{\varepsilon \to 0} \binom{k}{j} \frac{\Gamma\left(\frac{1}{2} + \frac{j}{2} + \frac{m}{2}\right) \Gamma\left(-\frac{j}{2} + k + \frac{m}{2} + r\right)}{2^{r} \Gamma\left(\frac{k}{2} + \frac{m}{2} + r\right) \Gamma\left(\frac{1}{2} + \frac{k}{2} + \frac{m}{2} + r\right)} F\left(-\frac{j}{2}, \frac{1}{2} - \frac{j}{2}; \frac{1}{2} - \frac{j}{2} - \frac{m}{2} + \varepsilon; 1\right) \\ &= \lim_{\varepsilon \to 0} \binom{k}{j} \frac{2^{k+r+2\varepsilon-2} \Gamma\left(-\frac{j}{2} + k + r + \frac{m}{2}\right) \Gamma\left(m - 2\varepsilon + 1\right) \sin(\pi(2\varepsilon - m))}{(k+m+2r)! \Gamma\left(1 - \frac{j}{2} + \frac{m}{2} - \varepsilon\right) \sin\left(\pi\left(\frac{1}{2} - \frac{j}{2} - \frac{m}{2} + \varepsilon\right)\right) \sin\left(\pi\left(\frac{j}{2} - \frac{m}{2} + \varepsilon\right)\right)} \end{split}$$

 $<sup>^1\</sup>mathrm{This}$  nice proof was pointed out to us by Christian Krattenthaler and is considerably easier than our first one.

Now note that the limit of the sin-terms is always 2. Hence, we finally obtain

$$\frac{2^{k+r-1} \left(\frac{m-j+2}{2}\right)_{k+r-1}}{(m+1)_{k+2r-1}}$$

as proposed.

The proof for the case r = 0 runs along similar lines. The only difference is the singular term  $\binom{k}{j}$  in front. However, after integrating the Beta integrals we can rewrite the corresponding sum as

$$\binom{k}{j} + \sum_{\ell \ge 0} \frac{k!}{\ell!(\ell+1)!(k-2\ell-2)!} \\ \times \sum_{i\ge 0} (-1)^i \binom{\ell+1}{k} \frac{1}{2^{2\ell+2}} \binom{k-2\ell-2}{j-2i} \frac{\Gamma(m/2+j/2-i+1/2)\Gamma(\ell+1)}{\Gamma(\ell+m/2+j/2-i+3/2)} \\ = \sum_{\ell\ge -1} \frac{k!}{\ell!(\ell+1)!(k-2\ell-2)!} \\ \times \sum_{i\ge 0} (-1)^i \binom{\ell+1}{k} \frac{1}{2^{2\ell+2}} \binom{k-2\ell-2}{j-2i} \frac{\Gamma(m/2+j/2-i+1/2)\Gamma(\ell+1)}{\Gamma(\ell+m/2+j/2-i+3/2)} \\ = \sum_{i\ge 0} \frac{(-1)^i(1+j-2i)_{k-j+2i}}{2^{2i}(k-j)!i!(\frac{1}{2}-i+\frac{j}{2}+\frac{m}{2})_i} F\left(\frac{j}{2}-\frac{k}{2},\frac{1}{2}+\frac{j}{2}-\frac{k}{2};\frac{1}{2}+\frac{j}{2}+\frac{m}{2};1\right)$$

and proceed as above.

## Lemma 8. Set

(4.4)  

$$T(k,r,\rho;v,\xi) := \sum_{m\geq 0} \sum_{j=0}^{k} \binom{k}{j} \frac{2^{k+r-\rho-1} \left(\frac{m-j+2}{2}\right)_{k+r-\rho-1}}{(m+1)_{k+r-1}} \frac{(k-j)!}{(k-j-\rho)!} v^{j} \frac{\xi^{m}}{m!}$$

and

(4.5) 
$$S(k,r,\rho;v,\xi) := \sum_{\tau=0}^{r-\rho} (-1)^{r-\rho-\tau} \binom{r-\rho}{\tau} T(k,r,\rho+\tau;v,\xi).$$

Then

(4.6) 
$$T(k, r, \rho; v, \xi) = \sum_{\tau=0}^{r-\rho} {\binom{r-\rho}{\tau}} S(k, r, \rho + \tau; v, \xi)$$

and

(4.7) 
$$S(k,r,\rho;v,\xi) = \frac{k!}{(k-\rho)!} \sum_{a\geq 0} {r-\rho \choose 2a} \frac{(2a)!}{2^a a!} A_{a+\rho}(k-\rho;v,\xi).$$

In particular we have  $S(k,r,\rho;v,\xi) \ge 0$  and  $T(k,r,\rho;v,\xi) \ge 0$  if  $|v| \le 1$ .

**Remark 9.** If we set  $\tilde{T}(k, r, \rho; v, \xi) = \frac{1}{2}(T(k, r, \rho; v, \xi) + T(k, r, \rho; -v, -\xi))$  and  $\tilde{S}(k, r, \rho; v, \xi) = \frac{1}{2}(S(k, r, \rho; v, \xi) + S(k, r, \rho; -v, -\xi))$  then we have (of course) corresponding representations in terms of  $\tilde{A}_r(k; v, \xi)$  and also  $\tilde{S}(k, r, \rho; v, \xi) \ge 0$  and  $\tilde{T}(k, r, \rho; v, \xi) \ge 0$  if  $|v| \le 1$ .

*Proof.* First note that (4.5) and (4.6) are equivalent. Thus, it remains to prove (4.7) or equivalently

$$T(k,r,\rho;v,\xi) = \sum_{\tau=0}^{r-\rho} {r-\rho \choose \tau} \frac{k!}{(k-\rho-\tau)!} \sum_{a\geq 0} {r-\rho-\tau \choose 2a} \frac{(2a)!}{2^a a!} A_{a+\rho+\tau}(k-\rho-\tau;v,\xi).$$

By expanding both sides with respect to  $v^j \xi^m/m!$  this identity is equivalent to

$$\binom{k}{j} \frac{2^{k+r-\rho-1} \left(\frac{m-j+2}{2}\right)_{k+r-\rho-1}}{(m+1)_{k+r-1}} \frac{(k-j)!}{(k-j-\rho)!} \\ = \sum_{\tau,a \ge 0} \binom{r-\rho}{\tau} \frac{k!}{(k-\rho-\tau)!} \binom{r-\rho-\tau}{2a} \frac{(2a)!}{2^a a!} \binom{k-\rho-\tau}{j} \frac{2^{k+a-1} \left(\frac{m-j+2}{2}\right)_{k+a-1}}{(m+1)_{k+2a+\rho+\tau-1}}$$

By rewriting the sum over  $\tau$  of the right hand side in hypergeometric notation and by using (4.2) we get

$$\begin{split} &\sum_{a\geq 0} \frac{(r-\rho)!k!2^{k-1} \left(\frac{m-j+2}{2}\right)_{k+a-1}}{j!(k-\rho-j)!(r-\rho-2a)!a!(m+1)_{k+2a+\rho-1}} \\ &\times F\left(-(r-\rho-2a), -(k-\rho-j); m+k+2a+\rho; 1\right) \\ &= \sum_{a\geq 0} \frac{(r-\rho)!k!2^{k-1} \left(\frac{m-j+2}{2}\right)_{k+a-1}}{j!(k-\rho-j)!(r-\rho-2a)!a!(m+1)_{k+2a+\rho-1}} \\ &\times \frac{\Gamma(m+k+2a+\rho)\Gamma(m+2k+r-\rho-j)}{\Gamma(m+k+r)\Gamma(m+2k+2a-j)} \end{split}$$

Next this sum can be also written in hypergeometric notation. Further, a second use of (4.2) and some simplifications (using the duplication formula of the Gamma

functions) yield

$$\begin{aligned} \frac{k!2^{k-1}\left(\frac{m-j+2}{2}\right)_{k-1}m!\Gamma(m+2k+r-\rho-j)}{j!(k-\rho-j)!\Gamma(m+k+r)\Gamma(m+2k-j)} \\ & \times F\left(-\frac{r-\rho}{2}, -\frac{r-\rho-1}{2}; \frac{m+2k-j+1}{2}; 1\right) \\ = \binom{k}{j}\frac{(k-j)!2^{k-1}\left(\frac{m-j+2}{2}\right)_{k-1}\Gamma(m+2k+r-\rho-j)}{(k-\rho-j)!(m+1)_{k+r-1}\Gamma(m+2k-j)} \\ & \times \frac{\Gamma\left(k+\frac{m}{2}-\frac{j}{2}+\frac{1}{2}\right)\Gamma\left(k+\frac{m}{2}-\frac{j}{2}+r-\rho-1\right)}{\Gamma\left(k+\frac{m}{2}-\frac{j}{2}+\frac{r}{2}-\frac{\rho}{2}-\frac{1}{2}\right)\Gamma\left(k+\frac{m}{2}-\frac{j}{2}+\frac{r}{2}-\frac{\rho}{2}-1\right)} \\ = \binom{k}{j}\frac{2^{k+r-\rho-1}\left(\frac{m-j+2}{2}\right)_{k+r-\rho-1}}{(m+1)_{k+r-1}}\frac{(k-j)!}{(k-j-\rho)!}\end{aligned}$$

as proposed.

# 

# 5. Proof of Theorem 1

First we use the results of the previous section to obtain another representation for  $\psi(x)$ .

**Lemma 9.** Suppose that  $b_2 > b_3$  and set

$$\begin{split} A_{12} &= a_{12}\sqrt{x_2} = a_{12}\sqrt{\frac{x}{b_2}}, \\ A_{13} &= a_{13}\sqrt{x_3} = a_{13}\sqrt{\frac{x}{b_3}}, \\ v &= \frac{2A_{12}A_{13}}{A_{12}^2 + A_{13}^2}, \\ \xi &= a_{23}\sqrt{x_2x_3}, \\ w_1 &= \frac{(1-x_3)}{2}(A_{12}^2 + A_{13}^2), \\ w_2 &= \frac{x_3 - x_2}{2(1-x_3)} \\ \omega &= 1 - \frac{A_{13}}{A_{12}}v = \frac{A_{12}^2 - A_{13}^2}{A_{12}^2 + A_{13}^2}. \end{split}$$

Then for  $x \in ]0, b_3[$  we have

$$\begin{split} \psi(x) &= \frac{2e^{\lambda+\mu}}{x(1-x_3)} \sum_{k\geq 1} \frac{w_1^k}{k!(k-1)!} \sum_{r=0}^{k-1} \binom{k-1}{r} w_2^r \sum_{L\geq 0} \frac{(-\lambda)^L}{L!} \\ &\times \sum_{\rho=0}^{r+L} \binom{r+L}{\rho} \tilde{S}(k,r+L,\rho;v,\xi) \, \omega^{\rho}. \end{split}$$

Proof. With help of Proposition 2 and Lemma 6 we get

$$\begin{split} \psi(x) &= \frac{2e^{\lambda+\mu}}{x(1-x_3)} \sum_{k\geq 1} \frac{w_1^k}{k!} \sum_{r=0}^{k-1} \binom{k-1}{r} w_2^r \sum_{L\geq 0} \frac{(-\lambda)^L}{L!} \\ &\times \sum_{m\geq 0} \sum_{0\leq j\leq k, j\equiv m \bmod 2} \binom{k}{j} \binom{\frac{m-j}{2}+k-1}{k-1} \\ &\times \sum_{\rho=0}^{r+L} (-1)^\rho \binom{r+L}{\rho} 2^{k+r+L-\rho-1} \left(\frac{2k+m-j}{2}\right)_{r+L-\rho} \frac{(k-j)!}{(k-j-\rho)!} \\ &\times v^j \left(\frac{A_{13}}{A_{12}}v\right)^\rho \frac{\xi^m}{(m+k+r-1)!} \\ &= \frac{2e^{\lambda+\mu}}{x(1-x_3)} \sum_{k\geq 1} \frac{w_1^k}{k!(k-1)!} \sum_{r=0}^{k-1} \binom{k-1}{r} w_2^r \sum_{L\geq 0} \frac{(-\lambda)^L}{L!} \\ &\times \sum_{\rho=0}^{r+L} (-1)^\rho \binom{r+L}{\rho} \left(\frac{A_{13}}{A_{12}}v\right)^\rho \\ &\times \sum_{m\geq 0} \sum_{0\leq j\leq k, j\equiv m \bmod 2} \binom{k}{j} \frac{2^{k+r+L-\rho-1} \left(\frac{m-j+2}{2}\right)_{k+r+L-\rho-1}}{(m+1)_{k+r+L-1}} \frac{(k-j)!}{(k-j-\rho)!} v^j \frac{\xi^m}{m!} \\ &= \frac{2e^{\lambda+\mu}}{x(1-x_3)} \sum_{k\geq 1} \frac{w_1^k}{k!(k-1)!} \sum_{r=0}^{k-1} \binom{k-1}{r} w_2^r \sum_{L\geq 0} \frac{(-\lambda)^L}{L!} \\ &\times \sum_{\rho=0}^{r+L} (-1)^\rho \binom{r+L}{\rho} \left(\frac{A_{13}}{A_{12}}v\right)^\rho \tilde{T}(k, r+L, \rho; v, \xi) \end{split}$$

Finally by using (4.6) we directly derive the proposed representation.

Note that  $|v| \leq 1$ . Thus this lemma shows that  $\psi(x) \geq 0$  if  $\omega \geq 0$  and  $\lambda \leq 0$  or equivalently  $|A_{12}| \geq |A_{13}|$  and  $a_1(b_2 - b_3) + a_2b_3 - a_3b_2 \geq 0$ . This is satisfied by assumptions of Theorem 1. Hence we have proved Theorem 1 for  $x \in ]0, b_3[$ . The case  $x \in ]b_3, b_2[$  is done by exchanging indices 1 and 2 and  $b_3$  by  $b_2 - b_3$  (compare with Remark 7).

## 6. Appendix: the first conjecture

We provide a counter-example for the original version of the BMV-conjecture as stated in [2]. We work with the notations of Section 3. Given the matrices

$$A = \begin{pmatrix} 0 & \frac{\epsilon^2}{2} & \epsilon \\ \frac{\epsilon^2}{2} & 0 & -\epsilon \\ \epsilon & -\epsilon & 0 \end{pmatrix}$$

and

$$B = \left(\begin{array}{rrr} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{array}\right),$$

we define the signed measure  $\mu_1^{A,B}(dx)$  as inverse Laplace transform of the function

$$z \mapsto \langle e_1, \exp(A - zB)e_1 \rangle$$
.

In the notations of Section 3 we have  $b_1 = b_3 = 0$  and  $b_2 = 1$ . We calculate the sign of the absolutely continuous part of  $\mu_1^{A,B}$  asymptotically in  $\epsilon$  and show that we obtain a negative sign for small  $\epsilon$  and  $x \in ]0,1[$ . We apply the formulas in the sense of Remark 7. We notice that  $y_1 = y_3 = 1 - x$  for  $0 \le x \le 1$ , which leads to the formula

$$\phi(k_1, k_2, k_3, x) = \frac{1-x}{(n-1)!} \int_0^1 f((1-t)(1-x), x, t(1-x)) \frac{(1-t)(1-x)}{k_1} dt,$$

for trajectories  $\gamma$  and  $\gamma_1 = 1$ , hence by following the lines of the proof of Theorem 2 we obtain

$$\psi_1(x) = \sum_{\substack{\gamma \in C \\ n \ge 2, \gamma_1 = 1}} \phi(k_1, k_2, k_3, x) a_{12}^{l_{12}} a_{13}^{l_{13}} a_{23}^{l_{23}}.$$

We only have to calculate the following cases up to order  $\epsilon^4$ , where # denotes the number of possible paths  $\gamma$  with given  $l_{ij}$ , where we apply Lemma 5, hence  $k_1 = \frac{l_{12}+l_{13}}{2} \ge 1$  and  $2l_{12} + l_{13} + l_{23} \le 4$ . We leave away paths  $\gamma$  with  $k_2 = 0$ , since those cannot contribute to a density for  $x \in ]0, 1[$ . This leads to the following table,

$l_{12}$	$l_{13}$	$l_{23}$	#
2	0	0	$P_1(1,0,0) = 1$
1	1	1	$P_1(1,1,1) = 2$
0	2	2	$P_1(1,2,2) = 1$

associated to the paths 121; 1321, 1231; 13231 (see Lemma 5, 3. in the appropriate translation as in Remark 7). Hence we obtain up to order  $\epsilon^4$  the following density for the absolutely continuous part

$$\psi_1^{A,B}(x) = (1-x)(\frac{\epsilon^2}{2})^2 - 2(1-x)^2\epsilon^2\frac{\epsilon^2}{2}\frac{1}{2} + (1-x)^3\epsilon^4\frac{1}{6} + \mathcal{O}(\epsilon^5),$$

consequently

$$\frac{12\psi_1^{A,B}(x)}{\epsilon^4} = 3(1-x) - 6(1-x)^2 + 2(1-x)^3 + \mathcal{O}(\epsilon)$$

where we obtain a negative sign if x is near 0.

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