A HYPER-GEOMETRIC APPROACH TO THE BMV-CONJECTURE

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Abstract. We provide a representation of the (signed) BMV-measure by stochastic means and prove positivity of the respective measures in dimension $d = 3$ in several non-trivial cases by combinatorial methods.

1. Introduction and Results

We aim to provide a representation of the (signed) measure related to the Bessis-Moussa-Villani conjecture (in the sequel BMV) by stochastic methods and calculate non-trivial cases in dimension 3 by hyper-geometric methods.

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

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

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 $[0, \infty[$,*

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

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 [8]

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has been published, where several further references can be found). We quote from [10]: "The BMV conjecture would 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 [3]. 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 the end of the article [2]).

At first sight the following relations hold true:

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

$$\frac{d}{dz}\phi^{A,B}(z) = -\operatorname{tr}(\exp(A - zB)B)$$
$$\frac{d^2}{dz^2}\phi^{A,B}(z) = \operatorname{tr}\left(\int_0^1 \exp(-s(A - zB))B\exp(s(A - zB))Bds\exp(A - zB)\right)$$

for $z \geq 0$. Hence $-\frac{d}{dz}\phi^{A,B}(z) \geq 0$ and $\frac{d^2}{dz^2}\phi^{A,B}(z) \geq 0$ for $z \geq 0$.

Proof. The first assertion follows from the fact that the eigenvalues of $\exp(A - zB)$ are non-neagtive and the second from the derivative of the function exp off 0 (see for instance [7], 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

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

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 [5]) tells that a smooth function $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}$ is the Laplace-transform of a non-negative measure μ 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 λ_1, since the identity matrix commutes with A, B.
(3) $\mu^{A,B+\lambda_2 I_d} = \mu^{A,B}(. + \lambda_2)$ for $\lambda_2 \geq -b_{\min}$, 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 λ_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 non-negative, the Dyson expansion (see Section 2 for a stochastic proof) yields that the BMV-conjecture holds true.

In view of all these well-known facts (for more investigations in these directions see [4]), the first non-trivial case, which appears in lowest non-trivial dimension, is the following. Take $d = 3$, $B = diag(b_1, b_2, b_3)$ 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 provide a Feynman-Kac-type construction – by stochastic means – of the Dyson series. Since Feynman-Kac-type Theorems are often used to prove that a function is a Laplace transform, we were motivated to construct an appropriate

Markov process for the non-stochastic matrix A in order to prove a Feynman-Kac representation for $\phi^{A,B}$. From this representation we can deduce the Dyson expansion and we are able to deduce a "semantics" of the problem, however, we were not able to conclude the result directly. The proof of the Feynman-Kac Theorem can be found in the Appendix, its application in order to prove the Dyson expansion in Section 2, see Theorem 2.

In Section 3 we concentrate on the 3-dimensional case, where we meet an important combinatorial simplification, see 2.7, which then leads to a summation problem in the theorie of hyper-geometric series. Finally we are able to prove the following result.

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

(1) $\frac{|a_{12}|}{\sqrt{b_2 - b_1}} \geq \frac{|a_{13}|}{\sqrt{b_3 - b_1}}$ *and* $\frac{|a_{12}|}{\sqrt{b_2 - b_1}} \geq \frac{|a_{23}|}{\sqrt{b_2 - b_3}}$.

(2) $a_{11}(b_2 - b_3) + a_{22}(b_3 - b_1) + a_{33}(b_1 - b_2) \geq 0$.

Then the function $\phi^{A,B}(z) := \mathrm{tr}(\exp(A - zB))$ *is completely monotone and the BMV-conjecture holds. Furthermore the BMV-conjecture holds (trivially) if two of the three eigenvalues* b_1, b_2, b_3 *agree or* $a_{12}a_{13}a_{23} \geq 0$.

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) on page 3.*

Remark 2. *The two conditions in (1) are related to positivity 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 *and appears to be the same on both intervals.*

Remark 3. *The proof of Theorem 1 will be given in Section 5. We note, however, that the assertions of the last sentence can be proved immediately (the argument shows all trivial cases).*

Proof. Assume that $a_{12}a_{13}a_{23} \geq 0$, then we can make a change of coordinates such that $a_{ij} \geq 0$, for $i \neq j$ by multiplying two coordinates by -1. If $a_{ij} \geq 0$ holds for $i \neq j$, 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 $(U^T AU)_{23} = 0$ and $U^T BU = B$. The trace is invariant under rotations, so

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

hence we find ourselves in the first trivial case. □

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

In this section we fix $d \geq 2$ and a $d \times d$ hermitian matrix A. We shall construct a Markov process $(Y_t^{(\zeta,i)})_{0\leq t\leq 1} := (Z_t^{(\zeta,i)}, X_t^i)_{0\leq t\leq 1}$ for $(\zeta, i) \in S$, which leads via the Feynman-Kac formula (see Theorem 3 in the Appendix), to a representation of the BMV-measure $\mu^{A,B}$. The state space of this Markov process is $S := \mathbb{C} \times \{1, \dots, d\}$. We shall assume a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1}, P)$, which allows for the subsequent constructions. Later we shall identify this space with the polish space of càdlàg paths on $[0, 1]$ with values in S.

Let $(N_t)_{t\geq 0}$ be a standard Poisson process with $N_0 = 0$ and jump intensity $d - 1$ defined on and adapted to $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1}, P)$. We denote by $(T_m)_{m\geq 0}$ the jumping times of $(N_t)_{0\leq t\leq 1}$, i.e. $T_m := \inf\{0 \leq t \leq 1,\, N_t \geq m\}$, where the infimum over the empty set equals infinity. We shall denote by $(X_t)_{t\geq 0}$ the càdlàg-process starting in a uniformly distributed way at points in S, i.e. $P(X_0 = i) = \frac{1}{d}$, and having the properties,

$$T_m = \inf\{t \geq T_{m-1} \text{ with } X_t \neq X_{T_{m-1}}\} \tag{2.1}$$

$$P(X_{T_m} = k | X_{T_m -} = l) = \frac{1}{d-1} \tag{2.2}$$

for $m \geq 1$ and $k \neq l \in \{1, \dots, d\}$, i.e. the process jumps at Poissonian jumping times T_m in a uniformly distributed way to another state. Note that this process is stationary, i.e. $P(X_t = i) = \frac{1}{d}$ for each $0 \leq t \leq 1$ and $1 \leq i \leq d$.

We define for $0 \leq t \leq 1$

$$Z_t := a_{X_0 X_{T_1}} a_{X_{T_1} X_{T_2}} \dots a_{X_{T_{n-1}} X_{T_{N_t}}} = \prod_{i=1}^{N_t} a_{X_{T_{i-1}} X_{T_i}}.$$

where the product is almost surely well defined as $N_1 < \infty$ almost surely. The empty product is defined to be 1. We set

$$Y_t := (Z_t, X_t)$$

for $0 \leq t \leq 1$. Then $(Y_t)_{0\leq t\leq 1} := (Z_t, X_t)_{0\leq t\leq 1}$ is a process with càdlàg paths starting in a uniformly distributed way at $\{(1,1),\dots,(1,d)\}$ in S.

Remark 4. *We may and will choose the polish space of càdlàg paths on* $[0,1]$ *with values in* S *as probability space* Ω *with the Borel probability measure* P*, such that the coordinate process on* Ω *together with the canonical filtrations* $(\mathcal{F}_t)_{0\leq t\leq 1}$ *satisfy the above requirements. Hence the process is a well defined map on the* entire *probability space* Ω*, which will allow us to leave out the usual "almost surely" at several occassions.*

We define probability measures P^i on $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1})$ by conditioning on the event $X_0 = i$ for $i \in \{1,\dots,d\}$, i.e. $P^i := P(.|X_0 = i)$. With respect to the probability measures P^i we define, for $(\zeta, i) \in S$, a process $(Y_t^{(\zeta,i)})_{0\leq t\leq 1} := (Z_t^{(\zeta,i)}, X_t^i)_{0\leq t\leq 1}$ on $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1}, P^i)$ through

$$
\begin{aligned}
X_t^i &= X_t \\
Z_t^{(\zeta,i)} &= \zeta Z_t
\end{aligned}
$$

for $0 \leq t \leq 1$.

Proposition 2. *Let* A *be a hermitian* $d\times d$ *matrix. The family of processes* $(Y_t^{(\zeta,i)})_{0\leq t\leq 1}$ *on* $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{0\leq t\leq 1}, P^i)$ *for* $(\zeta,i)\in S$ *defines a Markov process with generator*

$$
\mathcal{A}f(\zeta,i) = \sum_{\substack{j=1\\ j\neq i}}^{d} (f(\zeta a_{ij}, j) - f(\zeta, i)).
$$

for all $f \in C(S,\mathbb{C})$ *and* $(\zeta,i)\in S$*, where* $C(S,\mathbb{C})$ *denotes the set of continuous functions on* S*.*

Proof. Fix $f \in C(S, \mathbb{C})$ and $(\zeta, i) \in S$, then

$$\begin{aligned}
&\frac{1}{t} E_{P^i}(f(Z_t^{(\zeta,i)}, X_t^i) - f(\zeta, i)) \\
&= \frac{1}{t} \sum_{k=0}^{\infty} E_{P^i}(f(Z_t^{(\zeta,i)}, X_t^i) - f(\zeta, i) | N_t = k) P(N_t = k) \\
&= \frac{1}{t} \frac{1}{d-1} \sum_{\substack{j=1 \\ j \neq i}}^{d} (f(\zeta a_{ij}, j) - f(\zeta, i)) \frac{(d-1)t}{1!} e^{-(d-1)t} + \frac{1}{t} O(t^2) \\
&\to \sum_{\substack{j=1 \\ j \neq i}}^{d} (f(\zeta a_{ij}, j) - f(\zeta, i)),
\end{aligned}$$

as $t \to 0$. □

The Feynman-Kac formula allows for a stochastic interpretation of the BMV-measure $\mu^{A,B}$. Fix $r \in \mathbb{C}^d$, then Theorem 3 asserts for functions $f^r(\zeta, i) := r_i \zeta$, for $(\zeta, i) \in S$, the following formula to calculate $\exp(t(A - zB))r$.

Corollary 1. *Given $r \in \mathbb{C}^d$, a hermitian $d \times d$ matrix A and a diagonal matrix B with non-negative entries $b_1, \ldots, b_n$, we have*

$$\begin{aligned}
&E\left(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds) f^r(Y_1) | X_0 = i\right) \\
&= E_{P^i}\left(\exp(\int_0^1 a(X_s^i)ds - z\int_0^1 b(X_s^i)ds) f^r(Y_1^{(1,i)})\right) \\
&\qquad = e^{-(d-1)}(\exp(A - zB)r)_i
\end{aligned}$$

holds true for all $z \in \mathbb{C}$ and $1 \le i \le d$. Here $a = (a_1, \ldots, a_n)$ denotes the (real) vector of diagonal elements of A.

This formula allows for an interpretation of $z \mapsto (\exp(A - zB)r)_i$ as Laplace transform of the random variable $\int_0^1 b(X_s)ds$ under the (signed) measure Q^i on Ω

$$\frac{dQ^i}{dP} = \frac{1}{P(X_0 = i)} \exp(\int_0^1 a(X_s)ds) f^r(Y_1) 1_{\{X_0 = i\}},$$

since $\int_0^1 b(X_s)ds$ appears linearly in $-z$ in the exponent.

Given a hermitian $d \times d$ matrix A and a diagonal matrix B with non-negative diagonal entries $b_1, \ldots, b_d$, we define an $\mathcal{F}_0$-measurable random variable f on $\mathbb{C} \times \{1, \ldots, d\} \times (\Omega, \mathcal{F}_0, P)$ to obtain a closed formula for the trace $z \mapsto \mathrm{tr}(\exp(A - zB))$, namely

$$f(\zeta, i) := d e^{d-1} \zeta \begin{cases} 1 \text{ if } X_0 = i \\ 0 \text{ if } X_0 \neq i \end{cases} \tag{2.3}$$

for $\zeta \in \mathbb{C}$ and $i = 1, \ldots, d$. By Corollary 1 and Definition (2.3) we obtain, using the notation of Theorem 1,

$$\begin{aligned} \phi^{A,B}(z) &= \sum_{i=1}^{d} \langle e_i, \exp(A - zB)e_i \rangle \\ &= \sum_{i=1}^{d} E_{P^i}(\exp(\int_0^1 a(X_s^i)ds - z\int_0^1 b(X_s^i)ds) f^{e_i}(Y_1)) e^{d-1} d\frac{1}{d} \\ &= \sum_{i=1}^{d} E(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds) f(Y_1) | X_0 = i) P(X_0 = i) \\ &= E\left(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds) f(Y_1)\right) \end{aligned} \tag{2.4}$$

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

We now derive a series representation of the measure $\mu^{A,B}$. The function $f(Y_1)$ can take non-zero values only at loops, i.e. $X_0 = X_1$. First we introduce the subset $\Omega_n \subset \Omega$ consisting of those paths which form **loops** in $\{1, \ldots, d\}$ on $[0,1]$ with precisely n jumps for $n \geq 2$, i.e. $\Omega_n := \{X_0 = X_1, N_1 = n\}$. We define the set $C_n \subset \{1, \ldots, d\}^n$ as image set of the path random variable

$$\begin{aligned} p_n &: \Omega_n \to \{1, \ldots, d\}^n \\ \omega &\mapsto (X_{T_1-}(\omega), \ldots, X_{T_n-}(\omega)) \end{aligned}$$

So the subset C_n of $\{1, \ldots, d\}^n$ is characterized as set of all n-tuples such that no neighbors are equal and the last element X_{T_n-} is different from the first one $X_{T_1-} = X_0$. We denote $C := \cup_{n \geq 0} C_n$. 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 $\mathrm{ord}(\gamma)$: for $\gamma \in C_n$ we define

$$\mathrm{ord}(\gamma) := a_{\gamma_1\gamma_2} a_{\gamma_2\gamma_3} \ldots a_{\gamma_{n-1}\gamma_n} a_{\gamma_n\gamma_1} \tag{2.5}$$

$$= \prod_{i<j} a_{ij}^{l_{ij}(\gamma)}. \tag{2.6}$$

The **characteristic** $\mathrm{char}(\gamma) = (k_1(\gamma), \ldots, k_d(\gamma))$ of a path $\gamma \in C_n$ is defined by the number $k_j(\gamma)$ of visits in state j

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

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

$$\frac{1}{2}\sum_{j\neq i} l_{ij}(\gamma) = k_i(\gamma), \tag{2.7}$$

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

We shall denote by Δ_n the n-simplex in $\mathbb{R}^{n+1}$, i.e. the set of vectors $(t_1,\dots,t_{n+1}) \in \mathbb{R}^{n+1}$ 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 λ_n, i.e. $\lambda_n(\Delta_n) = 1$. For $\gamma \in C_n$, we consider the set $p_n^{-1}(\gamma) \subset \Omega_n$. On $p_n^{-1}(\gamma)$ we consider the conditional probability $P_\gamma := P(.|p_n = \gamma)$ and the random variable

$$\mathrm{dur} : p_n^{-1}(\gamma) \to \Delta_n$$

via $\mathrm{dur} := (T_1, T_2 - T_1, \dots, T_n - T_{n-1}, 1 - T_n)$, which has a uniform distribution λ_n on the simplex Δ_n under P_γ. Indeed since the conditional distribution of $(T_1, T_2 - T_1, T_3 - T_2, \dots, T_n - T_{n-1})$ for $n \geq 1$ under the condition $N_1 = n$ is uniform, we can conclude the result, i.e.

$$\begin{aligned}
&P_\gamma(T_1 \in [t_1, t_1 + dt_1], T_2 - T_1 \in [t_2, t_2 + dt_2], \dots, T_n - T_{n-1} \in [t_n, t_n + dt_n]) \\
&= \frac{1}{\frac{1}{d}\frac{e^{-(d-1)}}{n!}} \frac{1}{d}\frac{1}{d-1} dt_1 (d-1) e^{-t_1(d-1)} \dots \frac{1}{d-1} dt_n (d-1) e^{-t_n(d-1)} e^{-(1-\sum_{i=1}^n t_i)(d-1)} \\
&\qquad = \frac{dt_1 \dots dt_n e^{-(d-1)} (d-1)^n \frac{1}{d}\frac{1}{(d-1)^n}}{\frac{1}{d}\frac{e^{-(d-1)}}{n!}} = n! dt_1 \dots dt_n
\end{aligned}$$

for $\sum_{i=1}^n t_i \leq 1$. Here we apply that set $p_n^{-1}(\gamma)$ for $\gamma \in C_n$ has probability

$$P(p_n^{-1}(\gamma)) = \frac{1}{d(d-1)^n}\frac{e^{-(d-1)}(d-1)^n}{n!} = \frac{1}{d}\frac{e^{-(d-1)}}{n!}. \tag{2.8}$$

On the simplex Δ_n 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 on Δ_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 $h_1, \dots, h_{n+1}$.

Theorem 2. *Let A be a hermitian matrix, B a diagonal matrix with non-negative, mutually different entries $b_1, \dots, b_d$. The diagonal elements of A are denoted by*

$a_1, \dots, a_d$. *Then the measure (see Definition 1)* $\mu^{A,B}$ *is a signed measure decomposing into an absolutely continuous and singular part*

$$\mu^{A,B}(dx) = \sum_{i=1}^{d} \exp(a_i)\delta_{b_i}(dx) + \psi^{A,B}(x)dx. \tag{2.9}$$

$\psi^{A,B}$ *is a piecewise continuous function with possible disconituities at* b_i *and with support in* $[\min_i b_i, \max b_i]$. *We have*

$$\psi^{A,B}(x) = \sum_{\gamma \in C} \phi(\gamma, x) a_{\gamma_1\gamma_2} \dots a_{\gamma_n\gamma_1}, \tag{2.10}$$

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

$$\phi(\gamma, x)dx := \frac{1}{n!}\eta^{a_{\gamma_1},\dots,a_{\gamma_n},a_{\gamma_1};b_{\gamma_1},\dots,b_{\gamma_n},b_{\gamma_1}}(dx) \tag{2.11}$$

for $\gamma \in C_n$.

Proof. We can decompose the Feynman-Kac formula (2.4) by the number of jumps N_1, which appear up to time 1. This leads to

$$\begin{aligned} &E(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds)f(Y_1)) \\ &= \sum_{n=0}^{\infty} E(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds)f(Y_1), N_1 = n), \end{aligned}$$

wherefrom we obtain the basic decomposition of regular and singular part. The probability of taking 0 jumps up to time 1 and starting at i is $\frac{e^{-(d-1)}}{d}$, which leads to the expression for the singular part of $\mu^{A,B}$ in (2.9) by the definition of f. Again by the definition of f , formula (2.4) and formula (2.8) we obtain that, for $n \geq 1$,

$$\begin{aligned} &E(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds)f(Y_1), N_1 = n) \\ &= \sum_{\gamma \in C_n} E(\exp(\int_0^1 a(X_s)ds - z\int_0^1 b(X_s)ds)f(Y_1)|p_n = \gamma)P(p_n = \gamma) \\ &= \sum_{\gamma \in C_n} E_{P_\gamma}(\exp(\int_0^1 a(X_s|_{p_n^{-1}(\gamma)})ds - z\int_0^1 b(X_s|_{p_n^{-1}(\gamma)})ds)f(Y_1|_{p_n^{-1}(\gamma)}))P(p_n = \gamma) \\ &= \sum_{\gamma \in C_n} \int_0^{\infty} \exp(-zx)\frac{1}{n!}\eta^{a_{\gamma_1},\dots,a_{\gamma_n},a_{\gamma_1};b_{\gamma_1},\dots,b_{\gamma_n},b_{\gamma_1}}(dx)\,\mathrm{ord}(\gamma) \end{aligned}$$

holds true. We have applied that f equals $de^{(d-1)}\,\mathrm{ord}(\gamma)$ on the set $p_n^{-1}(\gamma)$, since this set consists of loops with favorable path γ and Z_1 takes precisely the value $\mathrm{ord}(\gamma)$. In addition $de^{(d-1)}P(p_n^{-1}(\gamma)) = \frac{1}{n!}$.

We have to show that the measure $\eta^{a_{\gamma_1},\dots,a_{\gamma_n},a_{\gamma_1};b_{\gamma_1},\dots,b_{\gamma_n},b_{\gamma_1}}(dx)$ has a density, which can be seen from the fact that the intersection of Δ_n and the set $\{\sum_{i=1}^n b_{\gamma_i} t_i + b_{\gamma_1} t_{n+1} = x\}$ depends in a differentiable way on x. The sum starts with $n = 2$ since there are no loops with only one jump. $\square$

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 $121\dots$ or $212\dots$, the contributions in the above series are necessarily non-negative: indeed for a hermitian 2×2 matrix A we must have that $\operatorname{ord}(\gamma) \geq 0$ for all loops γ and the measures η 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. *Theorem 2 can also be derived from the well-known Dyson expansion (see for instance* [4]*). Still we believe that the stochastic reasoning underlying our proof has special merits: it leads us to a probabilistic and combinatorial point of view (see Section 3 "Stochastic Semantics").*

Remark 6. *We have formulated Theorem 2 for Hermitian matrices A as this is presently our natural framework. But it is clear that it may as well be formulated for general $d \times d$ matrices A.*

3. Stochastic Semantics

From now on we assume $d = 3$ and $b_1 = 0$, we shall write $a_i = a_{ii}$ for $i = 1, 2, 3$. In particular all matrices will be real from now on. From the point of view of stochastic processes we now have a dynamic picture of the problem to calculate the measure $\mu^{A,B}$: we consider paths with values in the set $\{1, 2, 3\}$, which are favorable in the sense that two neighboring elements are different and the last element is different from the first one. The combinatorics of these paths leads us to a particular way to sum up the series (2.10). We think about trajectories dynamically as loops on the vertices $\{e_1, e_2, e_3\}$ of the 2-simplex. The total times ξ_i, which the trajectory stays in state i during time $[0, 1]$, form an element of the 2-simplex. Only if $\sum_{i=1}^3 b_i \xi_i \in [x, x + dx]$, the trajectory contributes to the density $\psi^{A,B}(x)dx$.

We now 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 Δ_2 with $\sum_{i=1}^3 b_i \xi_i = x$

will be parametrized by

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

with real numbers $0 < x_2 \leq x_3 < 1$ 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** $\mathrm{char}(\gamma) = (k_1(\gamma), k_2(\gamma), k_3(\gamma))$ of a path $\gamma \in C$ is the number of visits in the points $1, 2, 3$. 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

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

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

Lemma 1. *The characteristic* $\mathrm{char}(\gamma) = (k_1(\gamma), k_2(\gamma), k_3(\gamma))$ *of a path* $\gamma \in C$ *and the powers* $(l_{12}(\gamma), l_{13}(\gamma), l_{23}(\gamma))$ *of the order* $\mathrm{ord}(\gamma)$ *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 (2.7) and solve it for l_{ij} given $\mathrm{char}(\gamma)$, 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 $\eta^{a_{\gamma_1},\dots,a_{\gamma_n},a_{\gamma_1};b_{\gamma_1},\dots,b_{\gamma_n},b_{\gamma_1}}$ at x.

Lemma 2. *For $k_1, k_2, k_3 \geq 0$ define a probability density f on Δ_2 (this time with respect to uniform distribution $\frac{1}{2}\lambda_2$ of total mass $\frac{1}{2}$) given through*

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

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 $k_i \geq 1$. We fix a path $\gamma \in C$ with characteristic $\operatorname{char}(\gamma) = (k_1, k_2, k_3)$*, $n := k_1 + k_2 + k_3$, and define $\gamma' = (\gamma_1, \ldots, \gamma_n, \gamma_1) \in \{1, \ldots, d\}^{n+1}$ and*

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

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 $i = 1, 2, 3$. Notice that the law of the real-valued random variable $\omega \mapsto b_2\xi_2(p_n(\omega)) + b_3\xi_3(p_n(\omega))$ under P_γ is $\eta^{a_{\gamma_1}, \ldots, a_{\gamma_n}, a_{\gamma_1}; b_{\gamma_1}, \ldots, \gamma_n, \gamma_1}(dx) = n!\phi(\gamma, x)dx$ (see formula 2.11) Then the following assertions hold true:

(1) *Assume $k_i \geq 1$, for $i = 1, 2, 3$, then the law of the random variable pr_γ has density*

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

with respect to the measure $\frac{1}{2}\lambda_2$ on Δ_2. Notice that the state appearing in γ_1 is counted twice in the density.

(2) *For $k_i \geq 1$, $i = 1, 2, 3$, and $x \in \,]0, b_3[$*

$$\phi(\gamma, x) = \frac{1}{(n-1)!}\sqrt{\frac{1}{b_2 b_3}}\int_0^1 \left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \\ \frac{x_2(1-t)}{k_2} \\ \frac{x_3 t}{k_3} \end{array} \right\} \tag{3.3}$$

$$f(1 - x_2) + t(x_2 - x_3), x_2(1 - t), x_3 t)\sqrt{x_2 x_3}dt \tag{3.4}$$

at $0 < x < b_3$, where the cases in $\{\}$ pertain to $\gamma_1 = 1, 2, 3$. Notice the relations $b_2 x_2 = b_3 x_3 = x$.

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

(4) *Assume $k_2 = 0$, and $x \in]0, b_3[$, then*

$$\phi(\gamma, x) = \frac{1}{(n-1)!}\frac{(k_1 + k_3 - 1)!}{(k_1 - 1)!(k_3 - 1)!}\left\{ \begin{array}{ll} \exp(a_1(1 - x_3) + a_3 x_3)\frac{(1-x_3)^{k_1} x_3^{k_3-1}}{k_1 b_3} & \textit{if } \gamma_1 = 1 \\ \exp(a_1(1 - x_3) + a_3 x_3)\frac{(1-x_3)^{k_1-1} x_3^{k_3}}{k_3 b_3} & \textit{if } \gamma_1 = 3 \end{array} \right. \tag{3.5}$$

and n is necessarily even.

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

(3.6)

$$\phi(\gamma, x) = \frac{1}{(n-1)!} \frac{(k_1+k_2-1)!}{(k_1-1)!(k_2-1)!} \begin{cases} \exp(a_1(1-x_2)+a_2x_2)\frac{(1-x_2)^{k_1}x_2^{k_2-1}}{k_1b_2} & \text{if } \gamma_1 = 1 \\ \exp(a_1(1-x_2)+a_2x_2)\frac{(1-x_2)^{k_2-1}x_2^{k_2}}{k_2b_2} & \text{if } \gamma_1 = 2 \end{cases}$$

and n *is necessarily even.*

Proof. Fix $\gamma \in C_n$ and let $\gamma' = (\gamma_1, \ldots, \gamma_n, \gamma_1)$. 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 Δ_2, hence the norming factor is correct (the actual form of f stems from pushing forward with pr_γ and simply observing that a sum of independent uniformly distributed variables leads to a β-distribution). In the chart π_{12} (projection from Δ_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 $\{(\xi_1, \xi_2) \in \mathbb{R}^2, \quad \xi_1, \xi_2 \geq 0, \ \xi_1 + \xi_2 \leq 1\}$.

$$\frac{1}{2}\int_{\Delta_2} f(\xi_1,\xi_2,\xi_3)\lambda_2(d\xi) = \beta(k_1,k_2,k_3)\int_0^1\int_0^{1-\xi_2} \xi_1^{k_1-1}\xi_2^{k_2-1}(1-\xi_1-\xi_2)^{k_3-1}d\xi_1 d\xi_2$$

$$= \beta(k_1,k_2,k_3)\int_0^1 \xi_2^{k_2-1}(1-\xi_2)^{k_1+k_3-1}\int_0^{1-\xi_2} \frac{\xi_1^{k_1-1}}{(1-\xi_2)^{k_1-1}}(1-\frac{\xi_1}{1-\xi_2})^{k_3-1}d(\frac{\xi_1}{1-\xi_2})d\xi_2$$

$$= \beta(k_1,k_2,k_3)\int_0^1 \xi_2^{k_2-1}(1-\xi_2)^{k_1+k_3-1}\int_0^1 \eta^{k_1-1}(1-\eta)^{k_3-1}d\eta d\xi_2$$

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

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_γ 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

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

Shrinking the side $\text{conv}\{e_1 + x_2(e_2 - e_1), e_1 + x_3(e_3 - e_1)\}$ to an infitesimal 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

$$\sqrt{\frac{1}{b_2b_3}}\sqrt{x_2x_3}dxdt.$$

Hence we can determine $\phi_n(\gamma, x)$ through equation (2.11) and formula (3.2) evaluated at $((1-x_2)+t(x_2-x_3), x_2(1-t), x_3t)$, for $t \in [0,1]$,

$$\begin{aligned} &P_\gamma(b_2\xi_2 \circ p_n + b_3\xi_3 \circ p_n \in [x, x+dx]) \\ &= \sqrt{\frac{1}{b_2b_3}}\sqrt{x_2x_3}dx\frac{1}{(n-1)!}\beta(k_1,k_2,k_3)\int_0^1 \left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \\ \frac{x_2(1-t)}{k_2} \\ \frac{x_3t}{k_3} \end{array} \right\} \\ &f(1-x_2+t(x_2-x_3), x_2(1-t), x_3t)dt. \end{aligned}$$

For the degenerate cases we perform the same program. We first calculate the density of the law of pr_γ if one of the k_i is zero, which is a density supported by one edge of the simplex Δ_2. Assume $k_3 = 0$. With respect to the uniform distribution with total mass 1 on the edge $\mathrm{conv}\{e_1, e_2\}$ of Δ_2 we obtain for $k_1, k_2 \geq 1$

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

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 $k \geq 0$ and obtain the following proposition:

Lemma 3. *For $\gamma \in C$ and $x \in]0, b_3[$, we obtain in the sense of Gamma-functions*

$$\begin{aligned} \phi(\gamma, x) = \frac{1}{(n-1)!}\sqrt{\frac{1}{b_2b_3}}\int_0^1 &\left\{ \begin{array}{c} \frac{(1-x_2)+t(x_2-x_3)}{k_1} \\ \frac{x_2(1-t)}{k_2} \\ \frac{x_3t}{k_3} \end{array} \right\} \\ &f(1-x_2+t(x_2-x_3), x_2(1-t), x_3t)\sqrt{x_2x_3}dt, \end{aligned}$$

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

Proof. For $k_i \geq 1$ 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 7. Hence the limit yields

$$\begin{aligned}
&\lim_{\alpha\downarrow 0}\frac{1}{(n-1)!}\frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!}\sqrt{\frac{1}{b_2b_3}}\frac{1}{\Gamma(\alpha)}\int_0^1\left\{\begin{array}{c}\frac{(1-x_2)+t(x_2-x_3)}{k_1} \text{ if } \gamma_1=1\\ \frac{x_3t}{k_3} \text{ if } \gamma_1=3\end{array}\right\}\\
&\qquad((1-x_2)+t(x_2-x_3))^{k_1-1}(x_2(1-t))^{\alpha-1}(x_3t)^{k_3-1}\sqrt{x_2x_3}dt\\
&=\frac{\exp(\lambda+\mu)}{(n-1)!}\frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!}\frac{1}{x_2}\sqrt{\frac{x_2x_3}{b_2b_3}}\left\{\begin{array}{ll}\frac{(1-x_3)^{k_1}x_3^{k_3-1}}{k_1} & \text{if } \gamma_1=1\\ \frac{(1-x_3)^{k_1-1}x_3^{k_3}}{k_3} & \text{if } \gamma_1=3\end{array}\right.\\
&\quad=\frac{\exp(\lambda+\mu)}{(n-1)!}\frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!}\left\{\begin{array}{ll}\frac{(1-x_3)^{k_1}x_3^{k_3-1}}{k_1b_3} & \text{if } \gamma_1=1\\ \frac{(1-x_3)^{k_1-1}x_3^{k_3}}{k_3b_3} & \text{if } \gamma_1=3\end{array}\right. ,
\end{aligned}$$

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

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 γ with fixed characteristic $\mathrm{char}(\gamma)$ (and varying the first entry γ_1) formulas (3.3)-(3.6) appear in a simpler form, which only depends on the characteristic. We define the density

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

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

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

$$\chi(k_1,k_2,k_3,x)=\sqrt{\frac{1}{b_2b_3}}\frac{1}{n!}\int_0^1 f(1-x_2+t(x_2-x_3),x_2(1-t),x_3t)\sqrt{x_2x_3}dt \tag{3.7}$$

in the sense of Gamma-functions.

Remark 7. *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 $\mathrm{char}(\gamma)=(k_1,k_2,k_3)$, $k_i\geq 1$, by the binomial theorem and the Beta integral that*

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

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

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

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

Proof of Lemma 3. 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 $\mathrm{char}(\gamma) = (k_1,k_2,k_3)$ the path with $\gamma_1 = i$ appear with relative frequency $\frac{k_i}{n}$, hence absolutely

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

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

$$\begin{aligned}\chi(k_1,k_2,k_3,x) &= \frac{1}{\#\{\gamma\in C: \quad \mathrm{char}(\gamma) = (k_1,k_2,k_3)\}}\sum_{\substack{\gamma\in C\\ \mathrm{char}(\gamma)=(k_1,k_2,k_3)}}\phi(\gamma,x)\\
&= \frac{1}{(n-1)!}\sqrt{\frac{1}{b_2b_3}}\int_0^1\Big(\frac{k_1}{n}\frac{(1-x_2)+t(x_2-x_3)}{k_1}+\\
&+\frac{k_2}{n}\frac{x_2(1-t)}{k_2}+\frac{k_3}{n}\frac{x_3t}{k_3}\Big)\\
&f(1-x_2+t(x_2-x_3),x_2(1-t),x_3t)\sqrt{x_2x_3}dt\\
&= \frac{1}{n!}\sqrt{\frac{1}{b_2b_3}}\int_0^1 f(1-x_2+t(x_2-x_3),x_2(1-t),x_3t)\sqrt{x_2x_3}dt.\end{aligned}$$

For $k_1 = 0$ we conclude directly. For $k_2 = 0$ we use

$$\begin{aligned}\chi(k_1,0,k_3,x) &= \frac{1}{(n-1)!}\frac{k_1}{n}\frac{(k_1+k_3-1)!}{k_1!(k_3-1)!}\frac{x_3^{k_3-1}(1-x_3)^{k_1}}{b_3}\exp(a_1(1-x_3)+a_3x_3)+\\
&+\frac{1}{(n-1)!}\frac{k_3}{n}\frac{(k_1+k_3-1)!}{(k_1-1)!k_3!}\frac{x_3^{k_3}(1-x_3)^{k_1-1}}{b_3}\exp(a_1(1-x_3)+a_3x_3)\\
&= \frac{1}{n!}\frac{(k_1+k_3-1)!}{(k_1-1)!(k_3-1)!}\frac{x_3^{k_3-1}(1-x_3)^{k_1-1}}{b_3}\exp(a_1(1-x_3)+a_3x_3)\end{aligned}$$

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 $0 \leq y_1 \leq y_3 \leq 1$ satisfying the relations

$$\begin{aligned} b_2 y_1 &= b_2 - x \\ (b_2 - b_3) y_3 &= b_2 - x. \end{aligned}$$

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

$$\frac{1}{\sqrt{b_2(b_2 - b_3)}} \sqrt{y_1 y_3} dx$$

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

(3.8)

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

in the sense of Gamma-functions.

Remark 8. *Notice that the case $x \in]b_3, b_2[$ is deduced from the case $x \in]0, b_2[$ by the permutation $1 \longleftrightarrow 2$ 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 8 it suffices to consider the interval $]0, b_3[$.

Proposition 3. *Suppose that $b_2 > b_3$. Then, for $x \in]0, b_3[$, we have*

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

The *proof* of Proposition 3 is just a direct combination of Remark 7, 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 3 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 γ in C with $k_1(\gamma) = k$, $l_{13}(\gamma) = l$, $l_{23}(\gamma) = m$ and $l \equiv m \bmod 2$ is given through*

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

If $l \not\equiv m \bmod 2$, then the number of paths vanishes.

Proof. From [6] we get that the generating function of $\mathrm{ord}(\gamma)$ of all paths γ with $\gamma_1 = 1$ is given by

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

Hence, if $P_1(k, l, m)$ denotes the number of paths γ 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 $l \equiv m \bmod 2$)

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

Finally, if we denote by $P(k, l, m)$ the total number of paths γ 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

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

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

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

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

We start with a lemma, where we use the identity

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

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

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

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

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

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

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. $\square$

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

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

where r a is non-negative integer.

Lemma 7. *We have*

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

and

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

where r a is positive integer.

Remark 9. *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

$$\begin{aligned}
\tilde{A}_r(k;v,\xi) &= \frac{1}{2}\left(A_r(k;v,\xi)+A_r(k;-v,-\xi)\right)\\
&=\sum_{m\geq 0}\sum_{0\leq j\leq k,\ j\equiv m \bmod 2}\binom{k}{j}\frac{2^{k+r-1}\left(\frac{m-j+2}{2}\right)_{k+r-1}}{(m+1)_{k+2r-1}}\,v^j\,\frac{\xi^m}{m!}.
\end{aligned}$$

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

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

and

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

where r a is positive integer.

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

$$\begin{aligned}&[v^j]\int_0^1\sum_{\ell\ge 0}\frac{k!}{\ell!(\ell+r-1)!(k-2\ell)!}(1+sv)^{k-2\ell}\left(\frac{1-v^2}{2}\right)^{\ell}\left(\frac{1-s^2}{2}\right)^{\ell+r-1}s^m\,ds\\&=\int_0^1\sum_{\ell\ge 0}\frac{k!}{\ell!(\ell+r-1)!(k-2\ell)!}\\&\qquad\times\sum_{i\ge 0}(-1)^i\binom{\ell}{i}\frac{1}{2^\ell}\binom{k-2\ell}{j-2i}s^{j-2i}\left(\frac{1-s^2}{2}\right)^{\ell+r-1}s^m\,ds\end{aligned}$$

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

$$\begin{aligned}&\int_0^1\sum_{\ell\ge 0}\frac{k!}{\ell!(\ell+r-1)!(k-2\ell)!}\\&\qquad\times\sum_{i\ge 0}(-1)^i\binom{\ell}{i}\frac{1}{2^{2i+r}}\binom{k-2\ell}{j-2i}t^{m/2+j/2-i-1/2}(1-t)^{\ell+r-1}\,dt\\&=\sum_{\ell\ge 0}\frac{k!}{\ell!(\ell+r-1)!(k-2\ell)!}\\&\qquad\times\sum_{i\ge 0}(-1)^i\binom{\ell}{i}\frac{1}{2^{2i+r}}\binom{k-2\ell}{j-2i}\frac{\Gamma(m/2+j/2-i+1/2)\Gamma(\ell+r)}{\Gamma(\ell+r+m/2+j/2-i+1/2)}\\&=\sum_{i\ge 0}\frac{(-1)^i(1+i)_{k-i}}{2^{2i+r}(j-2i)!(k-j)!(\frac{1}{2}+i+\frac{j}{2}+\frac{m}{2})_{i+r}}\\&\qquad\times F\left(\frac{j}{2}-\frac{k}{2},\frac{1}{2}+\frac{j}{2}-\frac{k}{2};\frac{1}{2}+\frac{j}{2}+\frac{m}{2}+r;1\right).\end{aligned}$$

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

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

[1] This nice proof was pointed out to us by Christian Krattenthaler and is considerably easier than our first one.

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

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

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

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

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

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

Then

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

and

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

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 10. *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

$$\begin{aligned} &T(k,r,\rho;v,\xi)\\ &=\sum_{\tau=0}^{r-\rho}\binom{r-\rho}{\tau}\frac{k!}{(k-\rho-\tau)!}\sum_{a\ge 0}\binom{r-\rho-\tau}{2a}\frac{(2a)!}{2^a a!}A_{a+\rho+\tau}(k-\rho-\tau;v,\xi).\end{aligned}$$

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

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

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

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

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

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

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*

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

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

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

Proof. With help of Proposition 3 and Lemma 6 we get

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

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 $a_1(b_2 - b_3) + a_2 b_3 - a_3 b_2 \geq 0$. 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 8).

6. Appendix: the Feynman-Kac formula

We shall work with a continuous-time Markov process on the state space $S = \mathbb{C} \times \{1, \ldots, d\}$ associated to the off-diagonal elements of a $d \times d$ matrix $A \in M_d(\mathbb{C})$ with complex entries. The non-zero diagonal elements of A and the "potential" B will appear in exponential functionals of the process. We denote $\mathbb{C}$-valued functions on the state space S by f. Given a matrix $A \in M_d(\mathbb{C})$ with zero diagonal, we associate a generator $\mathcal{A}$ of a pure-jump type process on S, namely

$$\mathcal{A}f(\zeta,i) = \sum_{\substack{j=1\\ j\neq i}}^{d} (f(\zeta a_{ij}, j) - f(\zeta, i)).$$

The resulting S-valued Markov process is denoted by $Y_t^{(\zeta,i)} := (Z_t^{(\zeta,i)}, X_t^{(\zeta,i)})$ with initial value $(\zeta, i) \in S$ and has the following properties.

Lemma 10. *The projection of $(Y_t^{(\zeta,i)})_{t\geq 0} =: (Z_t^{(\zeta,i)}, X_t^{(\zeta,i)})_{t\geq 0}$ onto the second component will be denoted by (X_t^i), since it does not depend on $\zeta \in \mathbb{C}$, and equals in distribution the $\{1,\ldots,d\}$-valued Markov process associated to the matrix G with entries $g_{ij} = 1$ for $j \neq i$ and $g_{ii} = 1 - d$ for $i, j = 1, \ldots, d$.*

Proof. Take a function f on S, which does not depend on the first component ζ, then we have

$$\begin{aligned}\mathcal{A}f(i) &= \sum_{j=1}^{d} (f(j) - f(i)) \\ &= (Gf)_i,\end{aligned}$$

where we can identify f with a vector in $\mathbb{C}^d$. □

Lemma 11. *Let $f^r : \mathbb{C} \times \{1,\ldots,d\} \to \mathbb{C}$ be the function*

$$f^r(\zeta, i) := \zeta r_i$$

for $(\zeta, i) \in S$ and $r \in \mathbb{C}^d$ (which may be identified with a linear map from $\mathbb{C}^d$ to $C(S,\mathbb{C})$), then

$$\mathcal{A}f^r = f^{(A-(d-1)1_d)r}.$$

Proof. Direct calculation of the generator $\mathcal{A}$ on functions f^r. □

Furthermore given a real valued function V^b on S of the form

$$V^b(\zeta, i) = b_i$$

for $(\zeta, i) \in S$ (playing the role of a "potential") and $b \in \mathbb{C}^d$, then we can define the multiplication operator (denoted again by V^b) and we obtain

$$V^b f^r = f^{Br},$$

where B denotes the diagonal matrix with entries $b_1, \ldots, b_d \in \mathbb{C}$.

The main assertion of this section is the Feynman-Kac formula for the family of Markov process $(Y_t^{(\zeta,i)})_{t\geq 0}$ for $(\zeta,i)\in S$. Since we do not want to go into the theory of Feller semigroups and maximal domains, we formulate the Feynman-Kac Theorem in a special case, i.e. on a finite dimensional domain of definition.

Theorem 3. *Let A be any $d\times d$ matrix with entries in $\mathbb{C}$ and diagonal elements $a_1,\dots,a_d$, let V^b be the multiplication operator for $b\in\mathbb{C}^d$ as defined above, then for $z\in\mathbb{C}$ the function,*

$$u_t^r(\zeta,i)=E\left(\exp(\int_0^t a(X_s^i)ds - z\int_0^t b(X_s^i)ds)f^r(Y_t^{(\zeta,i)})\right)$$

solves the following differential equation on $C(S,\mathbb{C})$ for initial value f^r, $r\in\mathbb{C}^d$, and all $t\geq 0$,

$$\frac{\partial}{\partial t}u_t = \mathcal{A}u_t + V^a u_t - zV^b u_t \tag{6.1}$$

$$u_0 = f. \tag{6.2}$$

On the other hand, for initial value $f=f^r$, the solution to the differential equation (6.1) is given by

$$t\mapsto e^{-t(d-1)}f^{\exp(t(A-zB))r},$$

hence

$$E\left(\exp(\int_0^t a(X_s^i)ds - z\int_0^t b(X_s^i)ds)f^r(Y_t^{(1,i)})\right)=e^{-t(d-1)}(\exp(t(A-zB))r)_i$$

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

Proof. The proof is done by the Markov property for the process $(Y_t^{(\zeta,i)})_{t\geq 0}$ with $(\zeta,i)\in S$: first we show that the following semigroup property holds:

$$u_{t_1+t_2}^r(\zeta,i)=E(\exp(\int_0^{t_2} a(X_s^i)ds - z\int_0^{t_2} b(X_s^i)ds)u_{t_1}^r(Y_{t_2}^{(\zeta,i)}))$$

for $t_1, t_2 \geq 0$. Indeed, the right hand side can be written by the Markov property

$$
\begin{aligned}
&E(\exp(\int_0^{t_2} a(X_s^i)ds - z\int_0^{t_2} b(X_s^i)ds)u_{t_1}^r(Y_{t_2}^{(\zeta,i)}))\\
&= E\left(\exp(\int_0^{t_2} a(X_s^i)ds - z\int_0^{t_2} b(X_s^i)ds)E(\exp(\int_0^{t_1} a(X_s^i)ds - \right.\\
&\qquad \left. -z\int_0^{t_1} b(X_s^{\tilde{i}})ds)f^r(Y_{t_1}^{(\tilde{\zeta},\tilde{i})}))|_{(\tilde{\zeta},\tilde{i})=Y_{t_2}^{(\zeta,i)}}\right)\\
&= E\left(\exp(\int_0^{t_2} a(X_s^i)ds - z\int_0^{t_2} b(X_s^i)ds)E(\exp(\int_{t_1}^{t_1+t_2} a(X_s^i)ds - \right.\\
&\qquad \left. -z\int_{t_1}^{t_1+t_2} b(X_s^i)ds)f^r(Y_{t_1+t_2}^{(\zeta,i)})|\mathcal{F}_{t_1})\right)\\
&= E(\exp(\int_0^{t_1+t_2} a(X_s^i)ds - z\int_0^{t_1+t_2} b(X_s^i)ds))f^r(Y_{t_1+t_2}^{(\zeta,i)}))\\
&= f_{t_1+t_2}^r(\zeta,i)
\end{aligned}
$$

for all $t_1, t_2 \geq 0$, $(\zeta, i) \in S$ and $r \in \mathbb{C}^d$. Furthermore $r \mapsto u_t^r(\zeta, i)$ is obviously linear in r for fixed $(\zeta, i) \in S$ and $t \geq 0$. Hence it is sufficient to calculate the derivative at $t = 0$. This leads to

$$
\begin{aligned}
\frac{d}{dt}|_{t=0}u_t^r(\zeta,i) &= a_i r_i \zeta - z b_i r_i \zeta + \mathcal{A}u_0^r(\zeta,i)\\
&= (\mathcal{A} + V^a - V^{zb})f^r(\zeta,i)\\
&= f^{(Ar-(d-1)r-zBr)}(\zeta,i).
\end{aligned}
$$

Hence $(u_t^r)_{t\geq 0, r\in\mathbb{C}^d}$ defines a strongly continuous semiflow on the space $\{f^r, r \in \mathbb{C}^d\}$ with generator $\mathcal{A} + V^a - zV^b$, which a fortiori coincides with the semiflow $t \mapsto e^{-t(d-1)}f^{\exp(t(A-zB))r}$. □

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