MULTIGRADED POINCARÉ SERIES FOR MIXED STATES OF TWO QUBITS AND THE BOUNDARY OF THE SET OF SEPARABLE STATES

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ABSTRACT. Let $\mathcal{M}$ be the set of mixed states and $\mathcal{S}$ the set of separable states of the two-qubit system. Its Hilbert space is the tensor product $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, and the group of local unitary transformations is $G = \text{SU}(2) \times \text{SU}(2)$ (ignoring the overall phase factor). Let $\mathcal{P}$ be the algebra of real polynomial functions on the space of all hermitian operators of trace 1 on $\mathcal{H}$. Let $\mathcal{P}^G \subseteq \mathcal{P}$ be the subalgebra of $G$-invariants. We compute its multigraded Poincaré series and verify that it is consistent with Makhlin’s list of 18 invariants. By using the recent result of Augusiak et al. we describe the boundary of $\mathcal{S}$ and show that its intersection with the (relative) interior of $\mathcal{M}$ is a smooth manifold.

1. Introduction

Let $\mathbb{C}^n$ be the Hilbert space (of column vectors) with the inner product $\langle x_1, x_2 \rangle = x_1^\dagger x_2$ and let $M_n$ be the algebra of complex $n \times n$ matrices. If $X, Y \in M_n$ then their inner product is defined by $\langle X, Y \rangle = \text{tr}(X^\dagger Y)$. Let $\mathfrak{su}(n)$ denote the Lie algebra of $\text{SU}(n)$, it consists of all traceless skew-hermitian matrices in $M_n$.

The quantum system that we consider is bipartite. Both parties are qubits, $\mathbb{C}^2$. It will be convenient to identify $\mathbb{C}^4$ with the tensor product $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, and $M_4$ with $M_2 \otimes M_2$. For $X_1, X_2, Y_1, Y_2 \in M_2$, the inner product of $X_1 \otimes Y_1$ and $X_2 \otimes Y_2$ is given by $\langle X_1 \otimes Y_1, X_2 \otimes Y_2 \rangle = \langle X_1, X_2 \rangle \cdot \langle Y_1, Y_2 \rangle$.

It follows that $(X \otimes Y)^\dagger = X^\dagger \otimes Y^\dagger$ and, in particular, the tensor product of hermitian matrices is again a hermitian matrix.

The space of hermitian matrices $H_4 \subseteq M_4$ is the direct sum of the 1D real space spanned by the identity matrix, $I_4$, and the space $H_{4,0} = i\mathfrak{su}(4)$. The space $H_{4,0}$ is the direct sum of three real subspaces: $V_1 = H_{2,0} \otimes I_2$, $V_2 = I_2 \otimes H_{2,0}$, and $V_3 = H_{2,0} \otimes H_{2,0}$. Any mixed state, $\rho$, of our quantum system can be written uniquely as the sum of four components:

\begin{equation}
\rho = \frac{1}{4} I_4 + X \otimes I_2 + I_2 \otimes Y + Z,
\end{equation}

where $X, Y \in H_{2,0}$ and $Z \in V_3$.

Denote by $G$ the group of local unitary transformations, $\text{SU}(2) \times \text{SU}(2)$, where we ignore the overall phase factor. Note that $G$ acts on $M_4$ in the usual manner: $(g, Z) \rightarrow gZg^\dagger$ and stabilizes the real subspaces $H_4$ and $H_{4,0}$. Moreover, each of the subspaces $V_1, V_2, V_3$ is a simple $G$-module.

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Let $\mathcal{P}$ denote the algebra of real valued polynomial functions on $H_{4,0}$ and $\mathcal{P}^G$ the subalgebra of $G$-invariant functions. Note that $\mathcal{P}^G$ inherits the $\mathbb{Z}$-gradation from $\mathcal{P}$. The homogeneous polynomials of $\mathcal{P}^G$ may be used to construct measures of entanglement of our quantum system.

The knowledge of $\mathcal{P}^G$ is important because of the following well known fact: Two states, say $\rho_1$ and $\rho_2$, belong to different $G$-orbits iff there exists $f \in \mathcal{P}^G$ such that $f(\rho_1) \neq f(\rho_2)$. If this holds true for a subalgebra $\mathcal{A} \subseteq \mathcal{P}^G$, then we say that $\mathcal{A}$ is complete.

The Poincaré series (also known as the Hilbert series) of $\mathcal{P}^G$ was computed by M. Grassl et al. [4, Section VI]. We have

$$P(z) = \sum_{d=0}^{\infty} \dim(\mathcal{P}^G_d) z^d,$$

where $\mathcal{P}^G_d$ is the space of homogeneous polynomial $G$-invariants of degree $d$. This Poincaré series is a rational function of the variable $z$:

$$(1.2) \quad P(z) = \frac{1 - z^2 - z^3 + 2 z^4 + 2 z^5 + 2 z^6 - z^7 - z^8 + z^{10}}{(1 - z)^9 (1 + z)^6 (1 + z^2)^2 (1 + z + z^2)^3}.$$  

We remark that in [4] the formula contains an extra factor $1 - z$ in the denominator because the authors work with the space $H_4$ instead of $H_{4,0}$.

The Taylor expansion begins with

$$P(z) = 1 + 3 z^2 + 2 z^3 + 10 z^4 + 7 z^5 + 29 z^6 + 25 z^7 + 73 z^8 + 74 z^9 + 172 z^{10} + 187 z^{11} + 381 z^{12} + 431 z^{13} + 785 z^{14} + 920 z^{15} + 1539 z^{16} + 1827 z^{17} + 2878 z^{18} + 3441 z^{19} + 5151 z^{20} + 6185 z^{21} + 8887 z^{22} + 10666 z^{23} + \cdots$$

Subsequently, Y. Makhlin [8] gave a simple construction of 18 invariants which generate a complete subalgebra of $\mathcal{P}^G$. This subalgebra is proper and he gives two additional invariants. However, it is still not established whether this enlarged subalgebra is in fact the whole algebra $\mathcal{P}^G$. (According to M. Grassl [3] this can be proved by using the relations for the invariant tensors of SU(2).)

As a complement to the two papers just mentioned, we compute in Section 2 the $\mathbb{Z}^3$-graded Poincaré series of $\mathcal{P}^G$. This multigraded series carries more information about the invariants than the simply graded one.

Let us recall that a mixed state is called separable if it can be represented as a convex combination of product states, and otherwise it is called entangled. Denote by $\mathcal{M}$ the set of all states and by $\mathcal{S}$ the set of all separable states. It is well known that these two sets are compact and convex, and have nonempty interior. By $\partial \mathcal{M}$ resp. $\partial \mathcal{S}$ we denote the boundary of $\mathcal{M}$ and $\mathcal{S}$, respectively.

In Section 3 we show that there is a natural way of decomposing the boundary $\partial \mathcal{S}$ into two pieces. Each of these pieces is a portion of a real algebraic hypersurface in the ambient affine space. In particular, it follows from our results that the intersection of $\partial \mathcal{S}$ with the relative interior of $\mathcal{M}$ is a smooth manifold.

2. The multigraded Poincaré series

The direct decomposition $H_{4,0} = V_1 \oplus V_2 \oplus V_3$ induces a $\mathbb{Z}^3$-gradation on $\mathcal{P}$ which is preserved by the action of $G$. If the space of homogeneous invariants of degrees $d_1$, $d_2$, $d_3$ (with respect to the coordinates of the three subspaces) has dimension...
The multigraded Poincaré series \( P(t_1, t_2, t_3) \) of the algebra \( \mathcal{P}^G \) of local unitary polynomial invariants of mixed states of two qubits is the rational function, whose numerator \( N(t_1, t_2, t_3) \) and denominator \( D(t_1, t_2, t_3) \) are given by:

\[
N = 1 - t_1 t_3^2 - t_2 t_3^2 + t_1 t_2 t_3^2 + t_1 t_2^2 t_3^3 + t_1 t_2 t_3^4 + t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4 + t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4
+ t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4 + t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4 + t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4 + t_1 t_2^2 t_3^4 + t_1 t_2 t_3^4

\]

\[
D = (1 - t_1^2)(1 - t_2^2)(1 - t_3^2)(1 - t_1 t_2 t_3)(1 - t_1 t_3^2)(1 - t_2 t_3^2)(1 - t_3^2)(1 - t_4^2).
\]

The theorem is proved by using the well-known Molien–Weyl formula. Following the recipe from \( \mathbb{P} \), we obtain that

\[
P(t_1, t_2, t_3) = \frac{1}{(2\pi i)^3} \int_{|z|=1} \int_{|y|=1} \int_{|x|=1} \frac{\varphi(x, y, z, t_1, t_2, t_3)}{\varphi(x, y, z, t_1, t_2, t_3)} \frac{dx \, dy \, dz}{x \, y \, z},
\]

where

\[
\varphi(x, y, z, t_1, t_2, t_3) = \frac{(1 - x^{-1})(1 - y^{-1})(1 - z^{-1})(1 - y^{-1}z^{-1})}{\psi(x, y, z, t_1, t_2, t_3)}
\]

and

\[
\psi = (1 - t_1)(1 - t_3^2)(1 - t_3^2)(1 - t_1 x^{-1})(1 - t_3 x^{-1})(1 - t_3 x^{-1})(1 - t_3 x^{-1})
\]

\[
(1 - t_3 y)(1 - t_3 x z)(1 - t_3 x y z)(1 - t_3 x y z)(1 - t_3 x y z)(1 - t_3 x y z)
\]

\[
(1 - t_3 x^{-1} y)(1 - t_3 x^{-1} y)(1 - t_3 x^{-1} y)(1 - t_3 x^{-1} y)(1 - t_3 x^{-1} y)
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\[
(1 - t_2 y)(1 - t_2 y)(1 - t_2 y)(1 - t_2 y)(1 - t_2 y)
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(1 - t_3 y)(1 - t_3 y z)(1 - t_3 y z)(1 - t_3 y z)(1 - t_3 y z)
\]

\[
(1 - t_2 z)(1 - t_2 z)(1 - t_2 z)(1 - t_2 z)(1 - t_2 z).
\]

The three integrations are to be performed over the unit circle in the counterclockwise direction assuming that \( |t_i| < 1 \). The computation was carried out by using Maple \( \mathbb{P} \).

After setting \( t_1 = t_2 = t_3 = z \) in \( P(t_1, t_2, t_3) \), the numerator and denominator acquire the common factor \((1 + z^2)(1 - z^3)\). After cancellation, we obtain exactly the Eq. \( \mathbb{P} \), i.e., we have \( P(z, z, z) = P(z) \).

By expanding \( P(t_1, t_2, t_3) \) in the Taylor series, we find that

\[
P = 1 + t_1^2 + t_2^2 + t_3^2 + t_1 t_2 t_3 + 2 t_3^2 + 2 t_2 t_3^2 + 2 t_3^2 + t_3^2 + t_1 t_2 t_3^2
+ 2 t_1 t_2 t_3^2 + t_1 t_2 t_3^2 + 2 t_3^2 + 2 t_1 t_2 t_3^2 + 2 t_3^2 + t_3^2 + t_1 t_2 t_3^2
+ 2 t_1 t_2 t_3^2 + 3 t_3^2 + 4 t_2 t_3^2 + 2 t_2 t_3^2 + t_3^2 + t_3^2 + t_1 t_2 t_3^2
+ 3 t_3^2 + 4 t_2 t_3^2 + 2 t_2 t_3^2 + t_3^2 + t_3^2 + t_1 t_2 t_3^2
+ 4 t_2 t_3^2 + 4 t_2 t_3^2 + 4 t_2 t_3^2 + t_3^2 + t_3^2 + 2 t_3^2 + 2 t_1 t_2 t_3^2
+ 4 t_1 t_2 t_3^2 + 2 t_1 t_2 t_3^2 + 2 t_1 t_2 t_3^2 + 2 t_1 t_2 t_3^2 + 2 t_1 t_2 t_3^2
+ t_1 t_2 t_3^2 + 2 t_1 t_2 t_3^2 \cdots
\]

To make the connection with the notation in Makhlin’s paper, we may assume that the components of his vectors \( s \) and \( p \) are the linear coordinates on \( V_1 \) and \( V_2 \), respectively, and the nine entries \( \beta_{ij} \) of his matrix \( \hat{\beta} \) are the coordinates on
V_3. Then it is easy to check that his list of invariants agrees with the information provided by the coefficients in the above Taylor expansion. For instance, the cubic terms in the above expansion are t^3_3 and t_1 t_2 t_3. They correspond to Makhlin’s invariants I_1 and I_{12}, respectively.

3. The boundary of the set of separable states

Using Makhlin’s notation, we write the components X, Y, Z in Eq. (1.1) as

\[ X = \frac{1}{2} \sum s_i \sigma_i, \quad Y = \frac{1}{2} \sum p_i \sigma_i, \quad Z = \sum_{i,j} \beta_{ij} \sigma_i \otimes \sigma_j, \]

where the \( \sigma_i \)'s are the Pauli matrices

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

In [8, Table 1] Makhlin lists his 18 invariants \( I_1, \ldots, I_{18} \). We shall need only 9 of them:

\[
\begin{align*}
I_1 &= \det \hat{\beta}, \\
I_2 &= \text{tr}(\hat{\beta}^T \hat{\beta}), \\
I_3 &= \text{tr}(\hat{\beta}^T \hat{\beta})^2, \\
I_4 &= s^2, \\
I_5 &= |s\hat{\beta}|^2, \\
I_7 &= \mathbf{p}^2, \\
I_8 &= |\hat{\mathbf{p}}|^2, \\
I_{12} &= s\hat{\mathbf{p}}, \\
I_{14} &= e_{ijk} e_{lmn} s_i p_l \beta_{jm} \beta_{kn},
\end{align*}
\]

where \( e_{ijk} \) is the Levi–Civita symbol.

In a recent paper [1] Augusiak et al. have shown that \( S \) is exactly the set of all states \( \rho \) satisfying the inequality \( \det \rho^\Gamma \geq 0 \), where \( \Gamma \) is the operator of partial transposition, say with respect to the second party. Denote by \( D \) the real algebraic hypersurface in the affine space \((1/4)I_4 + H_{4,0}\) given by the equation \( \det \rho = 0 \). Its image under \( \Gamma \), which we denote by \( D^\Gamma \), is defined by the equation \( \det \rho^\Gamma = 0 \).

Let us recall that \( \partial \mathcal{M} \) consists of all \( \rho \geq 0 \) (with \( \text{tr} \rho = 1 \) having at least one zero eigenvalue, and so \( \partial \mathcal{M} \subseteq \mathcal{D} \). This inclusion is in fact proper, i.e., \( \partial \mathcal{M} \) is only a small portion of the entire hypersurface \( \mathcal{D} \). By the Peres–Horodecki criterion [6] we know that \( \mathcal{S} = \mathcal{M} \cap \mathcal{M}^\Gamma \). Hence, \( \partial \mathcal{S} \) is the union of two pieces:

\[ \partial \mathcal{S} = (\mathcal{D} \cap \mathcal{M}^\Gamma) \cup (\mathcal{D}^\Gamma \cap \mathcal{M}). \]

The first of these pieces has been mentioned in the paper [13] of Verstraete et al.

The polynomial function \( \det \rho^\Gamma \) is an invariant of \( G \). We have found the following expression for it in terms of the above Makhlin’s invariants:

\[
\det \rho^\Gamma = \frac{1}{256} - \frac{1}{32}(4I_2 + I_4 + I_7) + \frac{1}{2}(4I_1 + I_{12}) + \frac{1}{16}(32I_5 - 16I_5 - 16I_8 - 16I_{14} - 16I_9 + I_2^2 + I_7^2 + 8I_2 I_4 + 8I_2 I_7 - 2I_4 I_7).
\]

There are many papers devoted to the study of the geometry of the sets \( \mathcal{M} \) and \( \mathcal{S} \), e.g. [5, 6, 10, 12, 13, 14]. It may be of interest to study the boundary \( \partial \mathcal{S} \) and the determinantal hypersurface \( \mathcal{D} \) in more detail. Let us say that a point \( \rho_0 \in \mathcal{D} \) is smooth if the gradient \( \nabla \det \rho \) does not vanish at \( \rho_0 \), and otherwise it is a singular point of \( \mathcal{D} \).

The next proposition is valid for any \( n \)-dimensional complex Hilbert space \( \mathcal{H} \). In this more general setting both \( \mathcal{D} \) and \( \mathcal{D}^\Gamma \) are hypersurfaces in the real affine space \((1/n)I_n + H_{n,0}\).
Proposition 3.1. A point $\rho_0 \in D$ is a singular point of the hypersurface $D$ if and only if $\rho_0$ has at least two zero eigenvalues.

Proof. Let us arrange the eigenvalues of $\rho_0$ in increasing order

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n = 1 - \sum_{k=1}^{n-1} \lambda_k$$

and observe that we must have $\lambda_n > 0$. Since the unitary group $U(n)$ preserves $D$ and maps singular points to singular points, we may assume that $\rho_0$ is in fact the diagonal matrix

$$\rho_0 = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{n-1}, 1 - \lambda_1 - \cdots - \lambda_{n-1}).$$

For an arbitrary $\rho$, the determinant expansion has the form

$$\det \rho = \rho_{11} \rho_{22} \cdots \rho_{n-1,n-1} (1 - \rho_{11} - \cdots - \rho_{n-1,n-1}) + P,$$

where each term of the polynomial $P$ is at least quadratic in the off diagonal entries of $\rho$. Hence in evaluating the gradient of $\det \rho$ at the point $\rho_0$ the polynomial $P$ makes no contribution at all, and it suffices to use just the first term of the above expansion, which is written explicitly. We deduce that $\rho_0$ is a singular point if and only if the following equations hold:

$$\frac{\partial \det \rho}{\partial \rho_{kk}}(\rho_0) = \lambda_1 \lambda_2 \cdots \hat{\lambda_k} \cdots \lambda_{n-1} (\lambda_n - \lambda_k) = 0, \quad 1 \leq k \leq n - 1$$

where the hat means that $\lambda_k$ should be omitted. It is easy to see that these equations are satisfied if and only if at least two of the eigenvalues are 0. \qed

Note that if $n = 2$ then it is impossible for both eigenvalues to be 0, which means that in this special case the hypersurface $D$ is smooth. Indeed, we have $\partial \mathcal{M} = D$, $D$ is a sphere, and $\mathcal{M}$ the corresponding solid 3-dimensional ball.

The following corollary follows immediately from the proposition.

Corollary 3.2. A point $\rho_0 \in D_\Gamma$ is a singular point of $D_\Gamma$ if and only if $\rho_0^\Gamma$ has at least two zero eigenvalues.

Let us return now to the case of two qubits. In that case we shall prove that the piece $D_\Gamma \cap \mathcal{M}^0$, where $\mathcal{M}^0$ denotes the relative interior of $\mathcal{M}$, contains no singular points of the hypersurface $D_\Gamma$, i.e., for each $\rho \in D_\Gamma \cap \mathcal{M}^0$, the operator $\rho^\Gamma$ has exactly one zero eigenvalue.

Theorem 3.3. The piece of the hypersurface $D_\Gamma$ contained in the (relative) interior of $\mathcal{M}$ is smooth.

Proof. Assume that a point $\rho_0 \in D_\Gamma \cap \mathcal{M}^0$ is a singular point of $D_\Gamma$. Then $\rho_0^\Gamma$ is a singular point of $D$ and so it has at least two zero eigenvalues. We shall now apply an argument of Sanpera et al. \[11\]. By their Theorem 2, the zero eigenspace of $\rho_0^\Gamma$ contains a product vector $|e, f\rangle$, and obviously we have

$$\langle e, f | \rho_0^\Gamma | e, f \rangle = 0.$$

But this expression is equivalent to

$$\langle e, f^* | \rho_0 | e, f^* \rangle = 0,$$

which is impossible since $\rho_0 \in \mathcal{M}^0$, and so $\rho_0 > 0$. This contradiction proves the theorem. \qed
The following corollary is obvious.

**Corollary 3.4.** The piece of the hypersurface $D$ contained in the (relative) interior of $M^\Gamma$ is smooth.

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