

# On the orbit space of unitary actions for mixed quantum states

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# The problem statement

Generic question:

“CLASSICALITY OR QUANTUMNESS” ?

Mathematical problem:

DESCRIPTION OF THE ENTANGLEMENT SPACE

# Space of states

- A complete information on a generic  $N$ -dimensional quantum system is accumulated in  $N \times N$  density matrix  $\varrho$ .
  - 1 self-adjoint:  $\varrho = \varrho^\dagger$ ,
  - 2 positive semi-definite:  $\varrho \geq 0$ ,
  - 3 Unit trace:  $\text{Tr}\varrho = 1$ ,
- The set  $\mathfrak{P}_+$ , of all possible density matrices, is the space of (mixed) quantum states.
- Equivalence relation on  $\mathfrak{P}_+$ , due to the adjoint action of  $SU(N)$  group

$$(\text{Ad } g)\varrho = g\varrho g^{-1}, \quad g \in SU(N),$$

defines the orbit space  $\mathfrak{P}_+ | SU(N)$  that comprises a physically relevant knowledge.

# Density matrix for binary composites

- Composition of two subsystems represented by the Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  defines **tensor product space**

$$\mathcal{H}_{A \cup B} = \mathcal{H}_A \otimes \mathcal{H}_B.$$

- The density matrix of joint system  $\rho$  acts on  $\mathcal{H}_A \otimes \mathcal{H}_B$
- For a binary system,  $N_1 \otimes N_2$ , the **Local Unitary (LU)** equivalence,  $\rho \sim \rho'$ , means

$$\rho' = SU(N_1) \times SU(N_2) \rho (SU(N_1) \times SU(N_2))^\dagger.$$

- The **LU** equivalence decomposes  $\mathfrak{P}_+$  into the **local orbits**. The union of these classes is customary to call as the “**entanglement space**”  $\mathcal{E}_n$ .

# Entanglement

A bipartite quantum system is **separable** if its density matrix can be written in the form

$$\rho = \sum_{j=1}^M q_j \rho_j^A \otimes \rho_j^B, \quad q_j \geq 0 \quad \sum_{j=1}^M q_j = 1.$$

where  $\rho_j^A$  and  $\rho_j^B$  are density matrices of the constituent systems.

Otherwise the bipartite system is **entangled**.

The property to be entangled (resp. separated) as well as the measure of entanglement is preserved by local unitary transformations.

*“The **entanglement** of a two-qubit system is a **non-local property** so that **measures of entanglement** should be **independent of all local transformations** of the two qubits separately. Since a mixed two-qubit system is described by its density matrix, its nonlocal entangling properties must be described by **local invariants** of the density matrix.”*

King & Welsh. Qubits and invariant theory. J. Phys: Conf. Series **30**, 1-8, 2006.

## $\mathfrak{P}_+$ as semialgebraic variety

- The set of all  $N \times N$  Hermitian matrices with unit trace is a manifold in hyperplane  $P \subset \mathbb{R}^{N^2}$
- The positive semi-definiteness

$$\varrho \geq 0,$$

restricts manifold further to a **convex  $(N^2 - 1)$ -dimensional body**

- Since all roots of the characteristic equation

$$\det |\lambda I - \varrho| = \lambda^N - S_1 \lambda^{N-1} + \dots + (-1)^N S_N = 0,$$

are real, for their non-negativity it is **necessary and sufficient** that

$$S_k \geq 0, \quad \forall k.$$

## Example: Pairs of 2-qubits

- The unit trace condition and semipositivity of  $\varrho$  define semialgebraic set

$$0 \leq S_k \leq 1, \quad k = 1, 2, \dots, N.$$

- For 2 qubit case,  $S_k$  are polynomials up to **fourth order in 15 variables**, e.g., in **Fano parameters**

$$\varrho = \frac{1}{4} \left( I_2 \otimes I_2 + \vec{a} \cdot \vec{\sigma} \otimes I_2 + I_2 \otimes \vec{b} \cdot \vec{\sigma} + c_{ij} \sigma_i \otimes \sigma_j \right).$$

- Parameters  $c_{ij}$  determine the **correlation matrix**  $c_{ij} = \|C\|_{ij}$

# Coefficients $S_k$ for two qubits

$$S_2 = 1 - \frac{1}{3} (a^2 + b^2 + c^2)$$

$$S_3 = 1 - (a^2 + b^2 + c^2) - 2 \left( c_1 c_2 c_3 - \sum_{i=1}^3 a_i b_i c_i \right),$$

$$S_4 = \left( 1 - (a^2 + b^2 + c^2) \right)^2 + 8 \left( c_1 c_2 c_3 - \sum_{i=1}^3 a_i b_i c_i \right) \\ - 2 \left[ 2 \left( a^2 b^2 + (a_i^2 + b_i^2) c_i^2 - \sum_{\text{cyclic}} a_i b_i c_j c_k \right) + (c^2)^2 - c_i^4 \right].$$

$c_1, c_2, c_3$  - singular numbers of correlation matrix  $C$

# Peres–Horodecki separability criterion

- **Peres–Horodecki separability criterion:**

The system is **in a separable state** iff **partially transposed density matrix**

$$\varrho^{T_B} = I \otimes T \varrho, \quad T - \text{transposition operator}$$

**satisfies the conditions for a density operator.**

- **Coefficients of the characteristic equation for  $\varrho^{T_B}$ :**

$$S_2^{T_B} = S_2,$$

$$S_3^{T_B} = S_3 - \frac{1}{4} \det(C),$$

$$S_4^{T_B} = S_4 + \frac{1}{16} \det(M),$$

- **$M = \varrho - \varrho_A \otimes \varrho_B$  – Schlienz & Mahler matrix,**  
 **$\varrho_A = \text{tr}_B \varrho$  and  $\varrho_B = \text{tr}_A \varrho$  – density matrices of subsystems  $A$ , and  $B$ .**

# 3-parameter family of 2-qubits states

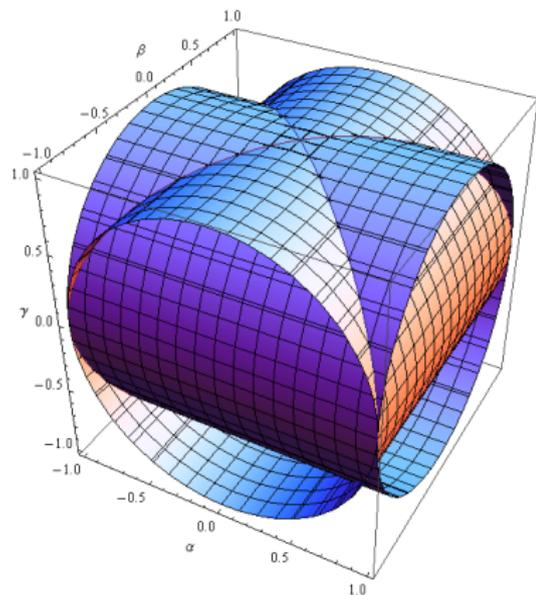
- A sample density matrix (GKP, Phys. Atom. Nucl. 74(6),893-900,2011)

$$\rho = \frac{1}{4} \begin{pmatrix} 1 + \alpha & 0 & 0 & 0 \\ 0 & 1 - \beta & i\gamma & 0 \\ 0 & -i\gamma & 1 + \beta & 0 \\ 0 & 0 & 0 & 1 - \alpha \end{pmatrix}$$

- Its **partially** transposed

$$\rho^{T_B} = \frac{1}{4} \begin{pmatrix} 1 + \alpha & 0 & 0 & i\gamma \\ 0 & 1 - \beta & 0 & 0 \\ 0 & 0 & 1 + \beta & 0 \\ -i\gamma & 0 & 0 & 1 - \alpha \end{pmatrix}$$

# Semipositivity domains



- $\rho \geq 0$  :

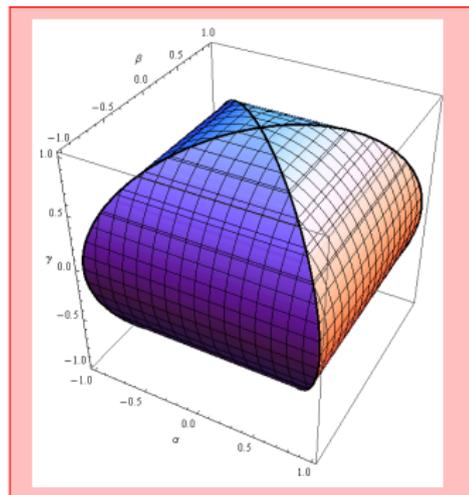
$$\alpha^2 \leq 1$$
$$\beta^2 + \gamma^2 \leq 1$$

- $\rho^{TB} \geq 0$  :

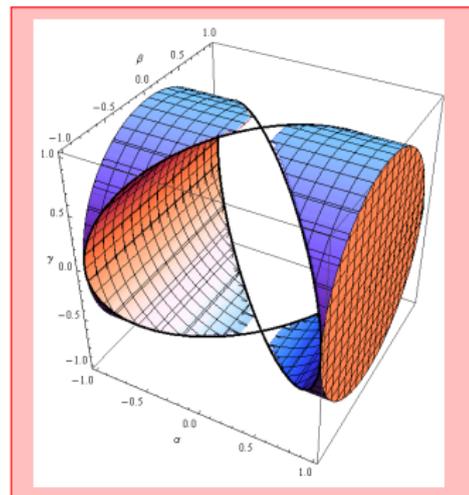
$$\beta^2 \leq 1$$
$$\alpha^2 + \gamma^2 \leq 1$$

# Domains of Separability vs. Entanglement

Separability domain



Entanglement domain



## Bipartite ( $r \times s$ -dimensional) quantum system

$$\rho = \frac{1}{r \cdot s} \left( \mathbb{I}_{r \cdot s} + \sum_{i=1}^{r^2-1} a_i \lambda_i \otimes \mathbb{I}_s + \sum_{i=1}^{s^2-1} b_i \mathbb{I}_r \otimes \mu_i + \sum_{i=1}^{r^2-1} \sum_{j=1}^{s^2-1} c_{ij} \lambda_i \otimes \mu_j \right)$$

$\rho$  is an element in the universal enveloping algebra of  $\mathfrak{su}(r \cdot s)$ .

Matrix  $C := \|c_{ij}\|$

$$c_{ij} = \text{Tr}(\rho \cdot \lambda_i \otimes \mu_j)$$

accounts for correlations of parts.

**Local unitary transformations:**

$$\rho \mapsto (U_1 \times U_2) \cdot \rho \cdot (U_1 \times U_2)^\dagger, \quad U_1 \in \text{SU}(r), \quad U_2 \in \text{SU}(s)$$

It is natural to describe the orbit space in terms of elements in the **invariant ring**  $K[X]^G$

$$X := \{a_i, b_j, c_{ij} \mid 1 \leq i \leq r^2 - 1, 1 \leq j \leq s^2 - 1\} \subset \mathbb{R}^{(r^2-1)(s^2-1)}$$

# Elements of Invariant Theory I

Let  $G$  be a **compact Lie group**. Then,

- The **invariant ring**

$$\mathbb{R}[X]^G := \{ p \in \mathbb{R}[X] \mid p(v) = p(g \circ v) \forall v \in V, g \in G \}$$

is finitely generated (**Hilbert's finiteness theorem**).

- There exist algorithms to construct generators of  $\mathbb{R}[X]^G$ .
- There exist a set of algebraically independent homogeneous **primary invariants**

$$\mathcal{P} := \{ p_1, \dots, p_q \} \subset \mathbb{R}[X]^G$$

such that  $\mathbb{R}[X]^G$  is integral over  $\mathbb{R}[\mathcal{P}]$  (**Noether normalization lemma**).

**Criterion:** the variety in  $C^q$  given by  $\mathcal{P}$  is  $\{0\}$ .

- There exist a set  $\mathcal{S} := \{ s_1, \dots, s_m \}$  of **secondary invariants**, homogeneous generators of  $\mathbb{R}[X]^G$  as a module over  $\mathbb{R}[\mathcal{P}]$ .

Together, primary and secondary invariants (**integrity basis**) generate  $\mathbb{R}[X]^G$ .

# Elements of Invariant Theory II

- $\mathbb{R}[X]^G$  is Cohen-Macaulay and there is a Hironaka decomposition

$$\mathbb{R}[X]^G = \bigoplus_{k=0}^m \mathfrak{s}_k \mathbb{R}[\mathcal{P}].$$

- **Orbit separation:** (Onishchik & Vinberg. Lie Groups and Algebraic Groups. Springer, 1990; Th.3, Chap.3, §4)

$$\forall u, v \in V \text{ s.t. } G \circ u \neq G \circ v : \exists p \in \mathbb{R}[X]^G \text{ s.t. } p(u) \neq p(v).$$

- **Syzygy ideal:**

$$I_{\mathcal{P}} := \{ h \in \mathbb{R}[y_1, \dots, y_q] \mid h(p_1, p_2, \dots, p_q) = 0 \text{ in } \mathbb{R}[x_1, \dots, x_d] \},$$

$$\mathbb{R}[y_1, \dots, y_q] / I_{\mathcal{P}} \simeq \mathbb{R}[X]^G.$$

# Algorithms to construct invariants of linear algebraic groups

- **Hilbert's algorithm**, 1893. Based on computing nullcone and then passing from invariants defining the nullcone to the complete set of generators, which amounts to an integral closure computation (Sturmfels. Algorithm in Invariant Theory. 2nd edition, 2008)
- **Derksen's algorithm** for reductive  $G$ , 1999. Implemented in **Magma**, **Singular**.
- Gattermann & Guyard, 1999. **Hilbert series driven Buchberger algorithm**.
- Bayer, 2003. **Algorithm for computation of invariants up to a given degree**. Implemented in **Singular**.
- Müller-Quade & Beth, 1999. Implemented in **Magma**.
- Hubert & Kogan, 2007. **Algorithm for computation of rational invariants**.
- .....
- Eröcal, Motsak, Schreyer, Steenpass, 2015 (arXiv:1502.01654v1 [math.AC]). Two refined **algorithms for computation of syzygies**. Implemented in **Singular**.

# Main Theorem

(Procesi & Schwarz. Invent. Math. 81,539-554,1985) (cf. also Abud & Sartori. Phys. Lett. B 104, 147-152,1981)

Let a compact Lie group  $G$  acts linearly on  $\mathbb{R}[X]$ ,  $\mathcal{B} = \{p_1, \dots, p_m\}$  be an integrity basis of  $\mathbb{R}[X]^G$  where  $X = \{x_1, \dots, x_d\}$  ( $\mathbb{R}[X]^G = \mathbb{R}[\mathcal{B}]$ ) and  $V_{\mathcal{B}} \subseteq \mathbb{R}^m$  be the real irreducible algebraic set (variety) generated by  $\mathcal{B}$ . Then  $\mathcal{B}$  defines the polynomial mapping

$$X \rightarrow \mathbb{R}[\mathcal{B}] : (x_1, \dots, x_d) \xrightarrow{p} (p_1, \dots, p_m),$$

such that

- The image  $Z \subseteq V_{\mathcal{B}}$  of  $p$  is a **semialgebraic set**.
- If one gives  $X$  and  $Z$  their classical topologies, then the mapping  $p$  is proper, and it induces a homomorphism

$$\bar{p}: X/G \rightarrow Z.$$

- $Z = \{v \in V_{\mathcal{B}} \mid \text{Grad}(v) \geq 0\}$ . where  $\text{Grad}$  is  $m \times m$  matrix

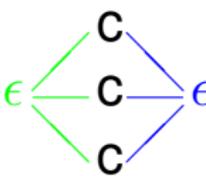
$$\|\text{Grad}\|_{\alpha\beta} = \partial_i p_{\alpha} \cdot \partial_i p_{\beta}.$$

The last positivity condition follows from  $(p_{\alpha} \partial_i p_{\alpha})(p_{\beta} \partial_i p_{\beta}) \geq 0$ .

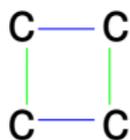
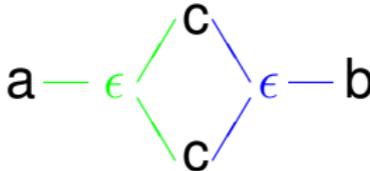
# Invariants for $SU(2) \times SU(2)$ I

King, Welsh, Jarvis. J. Phys. A: Math. Gen. 40, 10083-110108, 2007

2	$\mathbf{a} \text{---} \mathbf{a}$	$C_{200} = a_i a_i$
	$\mathbf{b} \text{---} \mathbf{b}$	$C_{020} = b_i b_i$
	$\mathbf{c} \text{---} \mathbf{c}$	$C_{002} = c_{ij} c_{ij}$

3	$\mathbf{a} \text{---} \mathbf{c} \text{---} \mathbf{b}$	$C_{111} = a_i b_j c_{ij}$
		$C_{003} = \frac{1}{3!} \epsilon_{ijk} \epsilon_{pqr} c_{ip} c_{jq} c_{kr}$

# Invariants for $SU(2) \times SU(2)$ II

4		$C_{202} = a_i a_j c_{i,\alpha} c_{j,\alpha}$
		$C_{022} = b_\alpha b_\beta c_{i,\alpha} c_{i,\beta}$
		$C_{004} = c_{i,\alpha} c_{i,\beta} c_{j,\alpha} c_{j,\beta}$
		$C_{112} = \frac{1}{2} \epsilon_{i,j,k} \epsilon_{\alpha,\beta,\gamma} a_j b_\alpha c_{j,\beta} c_{k,\gamma}$

5		$C_{113} = a_i b_\alpha c_{i,j} c_{k,j} c_{k,\alpha}$
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# Invariants for $SU(2) \times SU(2)$ III

6	$\begin{array}{ccc} a & \text{---} & c & \text{---} & c \\ & & & &   \\ a & \text{---} & c & \text{---} & c \end{array}$	$C_{204} = a_i a_\beta c_{i,j} c_{k,j} c_{k,\alpha} c_{\beta,\alpha}$
	$\begin{array}{ccc} b & \text{---} & c & \text{---} & c \\ & & & &   \\ b & \text{---} & c & \text{---} & c \end{array}$	$C_{024} = b_i b_\beta c_{j,i} c_{j,k} c_{\alpha,k} c_{\alpha,\beta}$
	$\begin{array}{cccc} a & \text{---} & \epsilon & \text{---} & c & \text{---} & b \\ & &   & & & & \\ & & c & \text{---} & c & \text{---} & a \end{array}$	$C_{213} = \epsilon_{i,j,k} a_i a_l b_\alpha c_{j,\alpha} c_{k,\gamma} c_{l,\gamma}$
	$\begin{array}{cccc} b & \text{---} & \epsilon & \text{---} & c & \text{---} & a \\ & &   & & & & \\ & & c & \text{---} & c & \text{---} & b \end{array}$	$C_{123} = \epsilon_{\alpha,\beta,\gamma} a_i b_\alpha b_\delta c_{i,\beta} c_{j,\gamma} c_{j,\delta}$

# Invariants for $SU(2) \times SU(2)$ IV

7	$  \begin{array}{cccc}  a & \text{---} \epsilon & \text{---} c & \text{---} b \\  &   & & \\  & c & \text{---} c & \text{---} c & \text{---} b  \end{array}  $	$C_{124} = \epsilon_{i,j,k} a_i b_\alpha b_\delta c_{j,\alpha} c_{k,\beta} c_{\gamma,\beta} c_{\gamma,\delta}$
	$  \begin{array}{cccc}  b & \text{---} \epsilon & \text{---} c & \text{---} a \\  &   & & \\  & c & \text{---} c & \text{---} c & \text{---} a  \end{array}  $	$C_{214} = \epsilon_{i,j,k} a_\alpha a_\delta b_i c_{\alpha,j} c_{\beta,k} c_{\beta,\gamma} c_{\delta,\gamma}$

8	$  \begin{array}{cccccc}  a & \text{---} \epsilon & \text{---} c & \text{---} c & \text{---} a \\  &   & & & \\  & c & \text{---} c & \text{---} c & \text{---} b  \end{array}  $	$C_{215} = \epsilon_{i,j,k} a_i a_\beta b_\eta c_{j,\alpha} c_{k,\gamma} c_{\beta,\alpha} c_{\delta,\gamma} c_{\delta,\eta}$
	$  \begin{array}{cccccc}  b & \text{---} \epsilon & \text{---} c & \text{---} c & \text{---} b \\  &   & & & \\  & c & \text{---} c & \text{---} c & \text{---} a  \end{array}  $	$C_{125} = \epsilon_{i,j,k} a_\eta b_i b_\beta c_{\alpha,j} c_{\gamma,k} c_{\alpha,\beta} c_{\gamma,\delta} c_{\eta,\delta}$

# Invariants for $SU(2) \times SU(2) \vee$

9		$C_{306} = \epsilon_{i,j,k} a_i a_\beta a_\theta c_{j,\alpha} c_{k,\gamma} c_{\beta,\alpha} c_{\delta,\gamma} c_{\delta,\eta} c_{\theta,\eta}$
		$C_{036} = \epsilon_{i,j,k} b_i b_\beta b_\theta c_{\alpha,j} c_{\gamma,k} c_{\alpha,\beta} c_{\gamma,\delta} c_{\eta,\delta} c_{\eta,\theta}$

## Example: 5-parameter density matrix (“X”-matrix)

$$\rho = \frac{1}{4} \begin{pmatrix} 1 + \alpha + \beta + \gamma_3 & 0 & 0 & \gamma_1 - \gamma_2 \\ 0 & 1 + \alpha - \beta - \gamma_3 & \gamma_1 + \gamma_2 & 0 \\ 0 & \gamma_1 + \gamma_2 & 1 - \alpha + \beta - \gamma_3 & 0 \\ \gamma_1 - \gamma_2 & 0 & 0 & 1 - \alpha - \beta + \gamma_3 \end{pmatrix}$$

**Fano parameters:**  $\mathbf{a}_3 = \alpha$ ,  $\mathbf{b}_3 = \beta$ ,  $\mathbf{c}_{11} = \gamma_1$ ,  $\mathbf{c}_{22} = \gamma_2$ ,  $\mathbf{c}_{33} = \gamma_3$

**Partial transposition:**

$$\rho^{T_b} = \frac{1}{4} \begin{pmatrix} 1 + \alpha + \beta + \gamma_3 & 0 & 0 & \gamma_1 + \gamma_2 \\ 0 & 1 + \alpha - \beta - \gamma_3 & \gamma_1 - \gamma_2 & 0 \\ 0 & \gamma_1 - \gamma_2 & 1 - \alpha + \beta - \gamma_3 & 0 \\ \gamma_1 + \gamma_2 & 0 & 0 & 1 - \alpha - \beta + \gamma_3 \end{pmatrix}$$

**Peres–Horodecki separability criterion:**

The two-qubit system is in a separable state iff partially transposed density matrix  $\rho^{T_b}$  satisfies the conditions for a density operator.

# Nonzero fundamental invariants

For our space of 5-parameter matrices there are 12 non-zero local invariants

$$C_{200}, C_{020}, C_{002}, C_{111}, C_{003}, C_{202}, C_{022}, C_{004}, C_{112}, C_{113}, C_{204}, C_{024}$$

of the form

$$\text{Deg 2 : } C_{200} = \alpha^2, \quad C_{020} = \beta^2, \quad C_{002} = \gamma_1^2 + \gamma_2^2 + \gamma_3^2$$

$$\text{Deg 3 : } C_{111} = \alpha\beta\gamma_3, \quad C_{003} = \gamma_1\gamma_2\gamma_3$$

$$\text{Deg 4 : } C_{202} = \alpha^2\gamma_3^2, \quad C_{022} = \beta^2\gamma_3^2$$
$$C_{004} = \gamma_1^4 + \gamma_2^4 + \gamma_3^4, \quad C_{112} = \alpha\beta\gamma_1\gamma_2$$

$$\text{Deg 5 : } C_{113} = \alpha\beta\gamma_3^3$$

$$\text{Deg 6 : } C_{204} = \alpha^2\gamma_3^4, \quad C_{024} = \alpha^2\gamma_3^4$$

# Primary invariants and syzygies

Primary invariants:

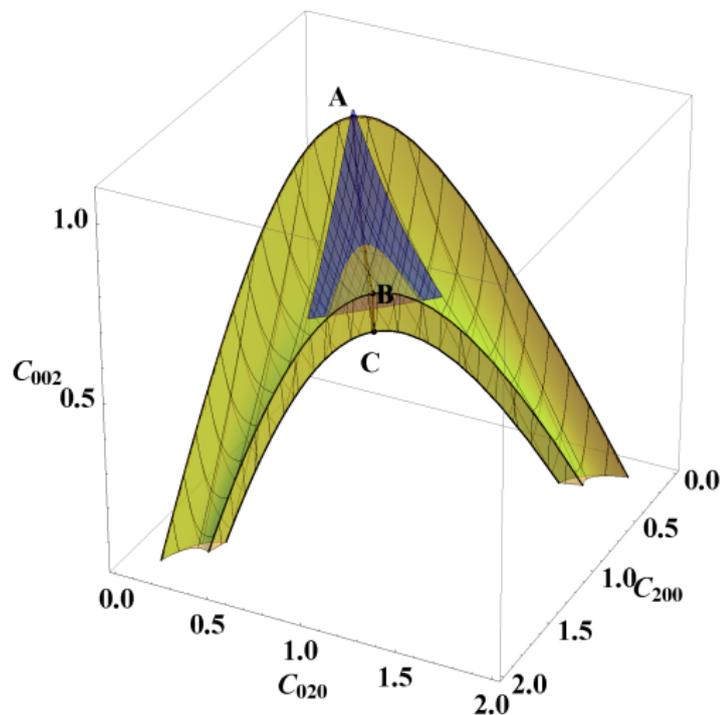
$$C_{200} \equiv a, \quad C_{020} \equiv b, \quad C_{002} \equiv c, \quad C_{111} \equiv x, \quad C_{003} \equiv y.$$

Solution of the syzygies

$$\begin{array}{lll} C_{204} = \frac{x^4}{ab^2} & C_{024} = \frac{x^4}{a^2b} & C_{112} = \frac{aby}{x} \\ C_{022} = \frac{x^2}{a} & C_{202} = \frac{x^2}{b} & C_{113} = \frac{x^3}{ab} \end{array}$$

$$C_{004} = c^2 + 2\frac{x^4}{a^2b^2} - 2\frac{cx^2}{ab} - 2\frac{aby^2}{x^2}$$

# Semipositivity of $\varrho$ and Grad



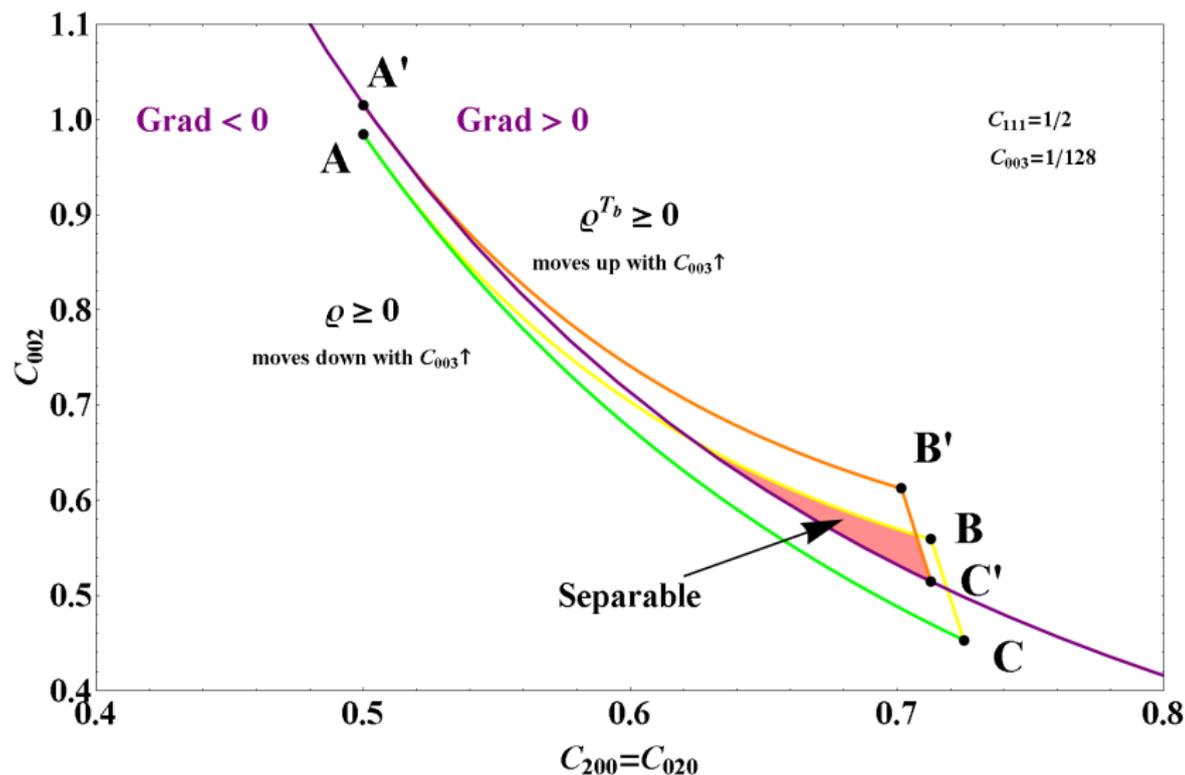
green:  $\varrho \geq 0$

blue:  $\text{Grad} \geq 0$

$C_{111} = 1/2,$

$C_{003} = 1/128$

# Separability area



# Conclusions

- It is natural to describe entanglement space of mixed quantum states in terms of local unitary invariants.
- The entanglement space is a semialgebraic variety.
- For 2-qubit the integrity basis of the invariant polynomial ring  $\mathbb{R}[X]^{SU(2) \times SU(2)}$  has been constructed. Here  $X$  is the set of 15 Fano parameters.
- It is a challenge for computer algebra to recompute algorithmically the integrity basis of  $\mathbb{R}[X]^{SU(2) \times SU(2)}$  and to derive the full set of polynomial equations and inequalities defining the 2-qubit entanglement space.
- Recent versions of MAPLE and MATHEMATICA have special built-in routines for (numerical) solving systems of polynomial equations and inequalities.