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# Classical positivity, quantum positivity and entanglement of a multi-partite density matrix, with the example of polarized reactions<sup>1</sup>

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**Abstract.** The spin correlations in a reaction involving initial and final polarized particles are encoded in a *cross section matrix* which is taken as an example of multipartite density matrix. *Quantum positivity* stipulates that the cross section is positive for any spin states - separable or entangled - of the particles. A weaker condition, *classical positivity* only requires that the cross section is positive for separable spin state. Classical and Quantum positivity are represented by diagrams. The domains of classical positivity and of separability are dual under a reciprocal polar transformation. This property can be useful in quantum information theory.

**Keywords:** entanglement ; positivity ; reciprocal polar transform

**PACS:** 32.60.+i , 13.88.+e

## INTRODUCTION

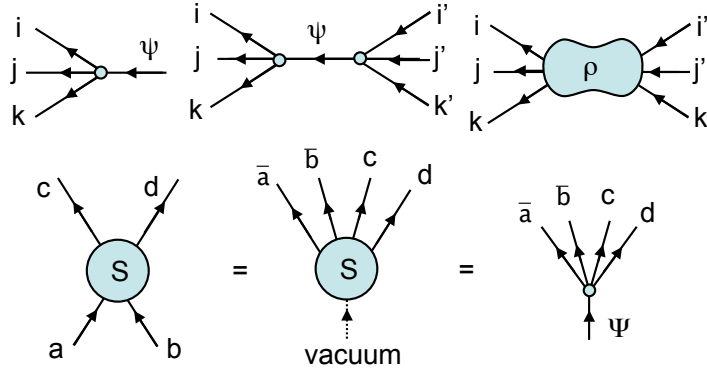
Density matrices of finite dimensions are basic objects in quantum information theory and in nuclear or high-energy spin physics. In the first field it is important to know if a given multi-partite density matrix is *separable* or *entangled*. In spin physics the attention is focused on the *positivity* constraints on the spin correlations [1]. These correlations are encoded in a *cross section matrix*  $\mathcal{R}$  which is a density matrix except for a trace differing from unity. In Ref. [1], some properties of  $\mathcal{R}$  related to quantum information, like entropy and entanglement are also discussed. In this paper we will review the concepts of *classical* and *quantum* positivity of  $\mathcal{R}$  introduced in Refs.[2, 1] with the help of graphical representations. We will also review a duality between the domains of separability and classical positivity of  $\mathcal{R}$ . This property can be useful in quantum information theory.

## STATES, DENSITY MATRIX AND S-MATRIX

We take the example of spin quantum states, but the results can be applied to any system containing quantum information of finite-dimension. To help the intuition, a graphical representation of states and operators is shown in Fig.1: a state  $\psi$  is represented by an oriented line, a density operator by a cocoon, the *S*-matrix by a disk and the scalar

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**FIGURE 1.** Upper row: graphical representation of a 3-particle wave function  $\langle i, j, k | \psi \rangle$ , a pure-state density matrix  $\langle i, j, k | \psi \rangle \langle \psi | i', j', k' \rangle$  and a mixed-state density matrix  $\langle i, j, k | \rho | i', j', k' \rangle$ . Lower row: representations of the equivalent quantities  $\langle c, d | S | a, b \rangle$ ,  $\langle \bar{a}, \bar{b}, c, d | S | \text{vacuum} \rangle$  and  $\langle \bar{a}, \bar{b}, c, d | \Psi \rangle$ .

product by a small bullet.  $|i\rangle, |j\rangle, |k\rangle, |a\rangle, |b\rangle$ , etc. are base vectors for the one-particle spin states (the base may differ from one particle to another). The upper row represents a 3-particle wave function  $\langle i, j, k | \psi \rangle$ , the corresponding density matrix which is of rank 1 and a mixed-state density matrix, of rank  $\geq 1$ .

The lower left diagram represents the  $S$ -matrix element  $\langle c, d | S | a, b \rangle$  of a polarized reaction  $A\uparrow + B\uparrow \rightarrow C\uparrow + D\uparrow$ . By *crossing* symmetry, it is equal to the  $S$ -matrix element  $\langle \bar{a}, \bar{b}, c, d | S | \text{vacuum} \rangle$  of the (fictitious) reaction  $\text{vacuum} \rightarrow \bar{A} + \bar{B} + C + D$ , shown in the lower middle. One can also write it as  $\langle \bar{a}, \bar{b}, c, d | \Psi \rangle$ , represented at the lower right, with  $|\Psi\rangle = S|\text{vacuum}\rangle$ . In the following  $|\Psi\rangle$  will be restricted to  $\bar{A} + \bar{B} + C + D$  spin states, excluding other sets of particles. It is then normalized to the unpolarized cross section:

$$\langle \Psi | \Psi \rangle = \sum_{a,b,c,d} |\langle c, d | S | a, b \rangle|^2 \propto (2s_A + 1)(2s_B + 1) \sigma(A + B \rightarrow C + D). \quad (1)$$

The crossing operation changes the spin variables  $a$  and  $b$  into  $\bar{a}$  and  $\bar{b}$ . However, re-labelling the spin bases of  $\bar{A}$  and  $\bar{B}$ , one can omit the bars and take  $\bar{a} = a, \bar{b} = b$ . Then

$$\langle c, d | S | a, b \rangle = \langle a, b, c, d | S | \text{vacuum} \rangle = \langle a, b, c, d | \Psi \rangle, \quad (2)$$

which reduces crossing to a *partial transposition*.

The *exclusive cross section matrix*, represented on the left of Fig.2, is  $\mathcal{R} = |\Psi\rangle \langle \Psi|$ . It is a pure-state density matrix (in this section we relax the condition that the trace of a density matrix is 1). Its matrix elements are given by

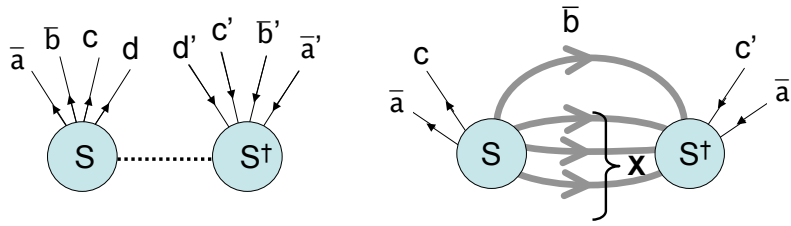
$$\langle a', b', c', d' | \mathcal{R} | a, b, c, d \rangle = \langle a', b', c', d' | S^\dagger | c', d' \rangle \langle c, d | S | a, b \rangle. \quad (3)$$

$\mathcal{R}$  encodes all polarization observables. The fully polarized cross section is

$$\sigma(A\uparrow + B\uparrow \rightarrow C\uparrow + D\uparrow) \propto \text{Tr} \{ \mathcal{R} (\rho_C \otimes \rho_D \otimes \rho_A^t \otimes \rho_B^t) \}. \quad (4)$$

The right diagram of Fig.2 represents the *semi-inclusive* cross section matrix when particles, which form the set  $\mathbf{X}$ , are undetected or when particles of known momenta are not polarized or not analyzed (here  $B$ ). This  $\mathcal{R}$  matrix is obtained from the exclusive one by taking the partial trace over unpolarized particles and integrating over the momenta of undetected particles. It is therefore a mixed-state density matrix.

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**FIGURE 2.** Graphical representations of the cross section matrix. Left: exclusive case. Right: semi-inclusive case. A summation over  $\bar{b}$  is understood.

## QUANTUM AND CLASSICAL POSITIVITY

In this section and the next one, the cross section matrix  $\mathcal{R}$  is taken as an example of a multipartite density matrix, except for the trace  $\neq 1$ .

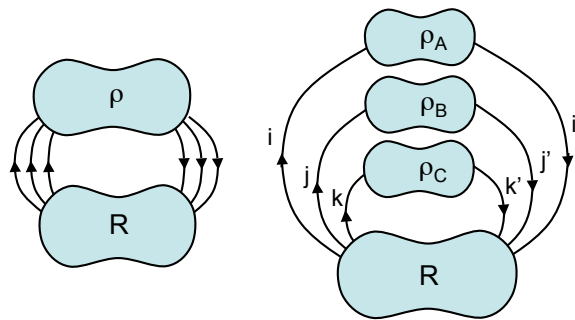
The  $\mathcal{R}$  matrix is *semi-positive definite*, that is to say  $\langle \varphi | \mathcal{R} | \varphi \rangle \geq 0$  for any, separable or entangled, multipartite spin state  $|\varphi\rangle$  (we will use the inexact but simpler word "positive"). Physically it means that the cross section is positive for all independent or entangled polarizations [1]. An equivalent statement is

$$\text{Tr} \{ \mathcal{R} \rho \} \geq 0 \quad \text{for any } \rho, \text{ separable or entangled.} \quad (5)$$

However, in ordinary collisions the particles are polarized or spin-analyzed independently, therefore what is experimentally verified is only the positivity of (4), which is equivalent to

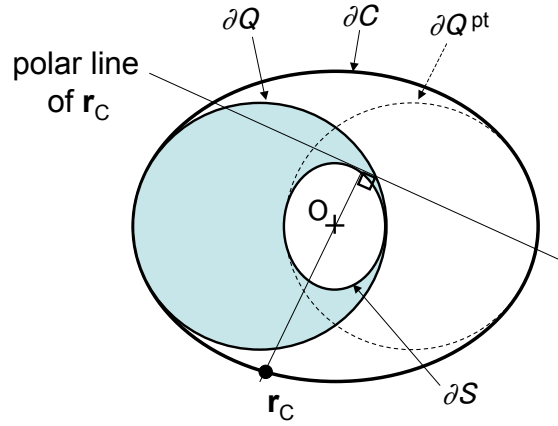
$$\text{Tr} \{ \mathcal{R} \rho \} \geq 0 \quad \text{for any separable } \rho. \quad (6)$$

This is the *classical positivity* condition. It is weaker than the *quantum positivity* condition (5). The traces in Eqs.(5) and (6) are represented on the left and right of Fig.3.



**FIGURE 3.** Graphical representations of the traces in Eq.(5) for quantum positivity (left) and Eq.(6) for classical positivity (right).

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**FIGURE 4.** Geometrical relationships between the domains of quantum positivity  $Q$ , classical positivity  $C$  and separability  $S$ . The dashed line is the boundary of the domain  $Q^{\text{pt}}$  where the partially transposed matrix is positive.

## POSITIVITY AND SEPARABILITY DOMAINS

In this section we assume that all density matrices have unit-traces.  $\mathcal{R}$  is renormalized accordingly. A density matrix can be parametrized as

$$\rho = (1 + \mathbf{r} \cdot \vec{\Sigma})/d \quad (7)$$

where  $d$  is the dimension of the quantum Hilbert space,  $\mathbf{r}$  a real vector of dimension  $D = d^2 - 1$  and the components  $\Sigma_1, \dots, \Sigma_D$  of  $\vec{\Sigma}$  are hermitian and traceless  $d \times d$  matrices satisfying

$$\text{Tr}(\Sigma_i \Sigma_j) = d \delta_{ij} \quad (8)$$

(this is a generalization of the spin-1/2 density matrix  $\rho = (1 + \mathbf{r} \cdot \vec{\sigma})/2$ ). Thus a density matrix is represented by a point in a  $D$ -dimensional Euclidean space. We have  $\text{Tr}(\rho \rho') = (1 + \mathbf{r} \cdot \mathbf{r}')/d$ . Setting  $\mathcal{R} \equiv \rho'$ , Eq.(5) tells that the domain  $Q$  of quantum positivity verifies

$$\mathbf{r} \cdot \mathbf{r}' \geq -1 \quad \text{for any } \mathbf{r} \text{ and } \mathbf{r}' \in Q. \quad (9)$$

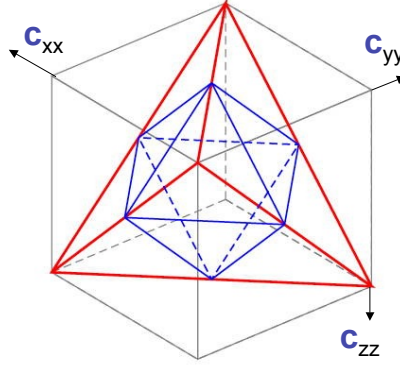
According to (6) the domain  $C$  of classical positivity is the largest one such that

$$\mathbf{r}_S \cdot \mathbf{r}_C \geq -1 \quad \text{for any } \mathbf{r}_S \in S \text{ and } \mathbf{r}_C \in C, \quad (10)$$

$S$  being the domain of separability.

$Q$ ,  $S$  and  $C$  are convex and  $S \subset Q \subset C$ . From (10) one can show that the boundaries  $\partial C$  and  $\partial S$  of  $C$  and  $S$  are dual in the *polar reciprocal transformation* of power  $-1$ . From (9) the boundary  $\partial Q$  of  $Q$  is self-dual. A two-dimensional picture of these relationships is shown in Fig.4, where a point  $\mathbf{r}_C$  of  $\partial C$  and its polar line  $\mathbf{r} \cdot \mathbf{r}_C = -1$ , which is tangent to  $\partial S$ , are drawn. The matrix  $\rho_C$  represented by  $\mathbf{r}_C$  is an *entanglement witness*, that is to say, a density matrix  $\rho$  verifying  $\text{Tr}(\rho \rho_C) < 0$  is certainly entangled. The matrices sitting on  $\partial C$  form a minimal complete set of entanglement witnesses.

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**FIGURE 5.** 3-dimensional projections of the domains of classical positivity  $C$  (cube), quantum positivity  $Q$  (tetrahedron) and separability  $S$  (octahedron).

Fig.4 also shows the boundary of the domain  $Q^{\text{pt}}$  where the partial transposed  $\rho^{\text{pt}}$  of  $\rho$  is positive.  $S$  and  $C$  are invariant under partial transposition.

As a precise example, let us consider the reaction  $A\uparrow + B\uparrow \rightarrow C + D$ , where  $A$  and  $B$  have spin 1/2 and the polarizations of  $C$  and  $D$  are not measured. The normalized  $\mathcal{R}$  matrix can be parametrized by

$$4\mathcal{R} = 1 + C_{x0}\sigma_x(A) + C_{y0}\sigma_y(A) + C_{z0}\sigma_z(A) + C_{0x}\sigma_x(B) + \dots \quad (11)$$

$$+ C_{xx}\sigma_x(A) \otimes \sigma_x(B) + C_{xy}\sigma_x(A) \otimes \sigma_y(B) + \dots \quad (12)$$

Let us focus on the three correlation coefficients  $C_{xx}$ ,  $C_{yy}$  and  $C_{zz}$ . Their 3-dimensional domain is contained the cube  $[-1, +1]^{\otimes 3}$  shown in Fig.5. Quantum positivity restricts this domain to the tetrahedron. It is the projection  $P(Q)$  of the positivity domain  $Q$  on the hyperplane  $\{C_{ij} = 0 \text{ for } i \neq j\}$ . Also shown are the projections  $P(C)$  and  $P(S)$  of the classical positivity and separability domains (the whole cube and the octahedron).

One can see that  $P(C)$  and  $P(S)$  are dual under the polar reciprocal transformation of power  $-1$  and that  $P(Q)$  is self-dual. This is a trace of the dualities of the non-projected domains. In fact, if two domains  $D_1$  and  $D_2$  are dual, the projection  $P(D_1)$  on a hyperplane  $H$  is dual to the intersection  $I(D_2)$  of  $D_2$  with  $H$ . In our example it happens that  $P(D) = I(D)$  for the three considered domains.

## CONCLUSION

We have shown that spin correlations in nuclear or high-energy physics provide useful examples in quantum information theory. More details can be found in Ref.[1]. The concept of classical positivity and its dual relationship with separability can help to find efficient entanglement criteria, for instance in quantum cryptography.

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