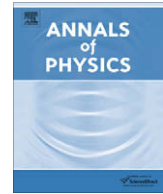




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Entanglement and the geometry of two qubits

J.E. Avron*, O. Kenneth

*Department of Physics, Technion, 32000 Haifa, Israel***ARTICLE INFO***Article history:*

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ABSTRACT

Two qubits is the simplest system where the notions of separable and entangled states and entanglement witnesses first appear. We give a three-dimensional geometric description of these notions. This description, however, carries no quantitative information on the measure of entanglement. A four-dimensional description captures also the entanglement measure. We give a neat formula for the Bell states which leads to a slick proof of the fundamental teleportation identity. We describe optimal distillation of two qubits geometrically and present a simple geometric proof of the Peres–Horodecki separability criterion.

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1. Introduction and overview

Geometric descriptions of physical notions are often both useful and elegant. For example, the geometric description of a single qubit¹ in terms of the Bloch sphere is a natural way of introducing the notion of a qubit [34] and at the same time is also a standard tool in the study of the polarization of photons [43].

Two qubits are the simplest setting where the notion of entanglement first appears. Our aim is to describe the world of two qubits geometrically. Algebraically, the world of two qubits is associated with 4×4 Hermitian matrices. This is a linear space of 16 dimensions. The large dimension makes it hard to visualize. To have a useful geometric description one needs to introduce appropriate equivalence relations which preserve the notions one wishes to describe while substantially reducing the dimension.

The fundamental notion of equivalence in quantum information reflects the freedom of all parties to independently choose bases for their Hilbert spaces. For a pair of qubits shared by Alice and Bob, this freedom is expressed by a pair of $SU(2)$ operations. Since $\dim SU(2) = 3$, this freedom corresponds

* Corresponding author. Fax: +972 4 8340 717.

E-mail address: avronj@gmail.com (J.E. Avron).

¹ D. Mermin [31] advocates the spelling “Qbit”.

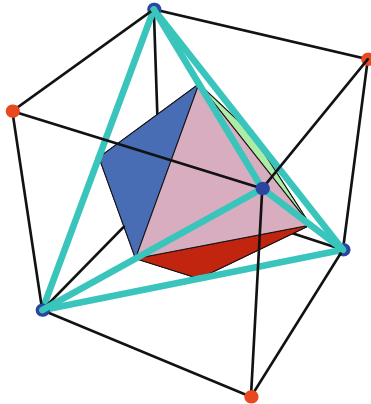


Fig. 1. The octahedron represents the equivalence class of separable states. The set of points that lie outside the octahedron but inside the tetrahedron represent the equivalence class of entangled states. The set of points that lie outside the tetrahedron but inside the cube represent entanglement witnesses. The vertices of the tetrahedron represent the equivalence class of pure states. Points related by the tetrahedral symmetry represent the same equivalence class.

to a six-dimensional family of unitary transformation. This reduces the 15 dimensions that describe the (normalized) states of two qubits to 9, which is still too large to be really useful.²

To further reduce the dimension one can allow Alice and Bob more freedom. The standard protocols of quantum information, such as local operation and classical communication (LOCC) [6] give Alice and Bob an arsenal of local operation: Besides the local unitary transformations they are also allowed to make local measurement and to communicate about what they did and what they got. They are not allowed to exchange qubits, however. In LOCC they are also not allowed to discard qubits but are allowed to do so in stochastic local operation and classical communication (SLOCC) [7]. This makes SLOCC a filtering process.

LOCC and SLOCC do not naturally lead to equivalence relations but rather to partial order. For example, it is a fundamental feature of entanglement, arguably its defining property, that entanglement cannot be created by local operations [38] although it can be locally degraded and destroyed.

We therefore need to introduce a different class of operations that can serve as an equivalence relation. *We shall consider two states as equivalent if each can be prepared from the other (filtered) with finite probability by local operations.* Unlike LOCC or SLOCC, this is a symmetric relation, and hence an equivalence. It restricts the local operations to those represented by invertible matrices [28,47]. In particular, Alice and Bob are not allowed to make projective measurement or mix pure qubits because these operations are not reversible, even probabilistically (more on this, below).

For describing *notions*, such as entanglement and witnesses, it is convenient to forget about the normalization of states. This allows one to describe the world of two qubits in three dimensions [28], as shown in Fig. 1. Interestingly, the same figure appears in various other contexts in quantum information theory. It first appeared in the Horodeckie’s description [24] of two qubits with maximally mixed subsystems. It also appears in the characterization of the capacity of a single qubit quantum channel [41,20,26,42,54] and in other contexts [1,49,21,45].

The three-dimensional description, beautiful as it is, has weaknesses. One is that there are certain (fortunately, non-generic) states that do not seem to fit anywhere in Fig. 1. An example is the family of states where at least one subsystem is pure

$$(\text{pure})_A \otimes (\text{mixed})_B, \quad (\text{mixed})_A \otimes (\text{pure})_B, \quad (\text{pure})_A \otimes (\text{pure})_B. \tag{1.1}$$

Another weakness is that the three-dimensional figure gives no information on the measure of entanglement: The distance from the octahedron does not reflect any of the accepted measures of entangle-

² There are, however, certain interesting lower-dimensional families of states for which the reduction is powerful enough [24].

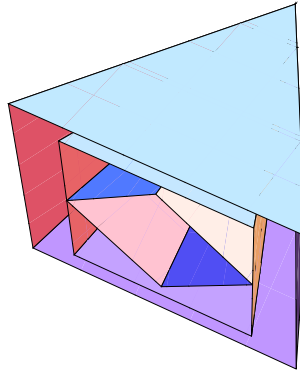


Fig. 2. Four-dimensional truncated cones describe the LSL equivalence classes of the of trace normalized witnesses, entangled and separable states. The cross-section of the cones, here represented by nested rectangles, are the three-dimensional polyhedra shown in Fig. 1. The largest cone is the cone of potential witnesses and the smallest cone is the dual cone of separable states. The intermediate cone is the self-dual cone of states. The distance from the cone of separable states is a measure of entanglement. The extraordinary families of Eq. (1.1) are represented by the apex of the cone.

ment [39]. This is a consequence of the fact that the normalization of states does not matter in the three-dimensional description.

To remedy this, we look at operations where the normalization of states matters. Specifically, we allow Alice and Bob to act on their qubits by matrices $M_{A,B} \in SL(2, \mathbb{C})$, the group of 2×2 matrices, with complex entries and unit determinant. The interpretation of this family in terms of measurements shall be discussed in Section 5. We shall call this class of operations LSL (for local, special and linear). LSL allows for a geometric description of the measure of entanglement. The price one pays is that one needs to go to four dimensions. The geometric picture that emerges is illustrated in Fig. 2, showing three nested cones. The largest cone is the cone of potential witnesses, whose cross-section is the cube in Fig. 1. The boundary of the cone is special in that it is cohabited by two inequivalent families: The ordinary and the extraordinary. This makes it pathological.³ It may seem odd that the world of two qubits, which is a simple linear space in 16 dimensions, becomes pathological when viewed in terms of its equivalence classes. A useful analogy is the partitioning of (the connected) Minkowsky space-time to the (disconnected) equivalence classes of time-like, light-like and space-like vectors.

The four-dimensional description is faithful to the measure of entanglement. More precisely, the concurrence, [51,52], is the distance from the cone of separable states, the smallest nested cone. In particular, states represented by points near the apex of the cone have very little entanglement.

Many things will have to be left out. Among them: the notions of “entanglement of formation”, “entanglement cost” [6,7,18]; “bound entanglement” [22], “entanglement persistence” [10], multipartities entanglement, GHZ states [16] and the different entanglement measures [39]. Comprehensive reviews of entanglement, with extensive bibliography, are [55,4,25].

2. Bell states

The mothers of all entangled states are the four Bell states [9], commonly denoted by $|\beta_\mu\rangle$, here chosen to be

$$\begin{aligned} \sqrt{2}|\beta_0\rangle &= |00\rangle + |11\rangle, & \sqrt{2}|\beta_1\rangle &= |00\rangle - |11\rangle, \\ \sqrt{2}|\beta_2\rangle &= |01\rangle + |10\rangle, & i\sqrt{2}|\beta_3\rangle &= |01\rangle - |10\rangle. \end{aligned} \tag{2.1}$$

³ When distinct points cannot be separated a space is non-Hausdorff.

The (isotropic) singlet is then $|\beta_3\rangle$. It is not a coincidence that the number of Bell states coincides with the number of Pauli matrices σ_μ (with σ_0 the identity).

Proposition 2.1. *The Pauli matrices give the unitary map from the computational basis, $|a\rangle \otimes |b\rangle$, with a, b binary, to the Bell basis $|\beta_\mu\rangle$, $\mu \in \{0, 1, 2, 3\}$. Explicitly:*

$$\sqrt{2}|\beta_\mu\rangle = (\sigma_\mu)_{ab}|a\rangle \otimes |b\rangle, \quad \sqrt{2}|a\rangle \otimes |b\rangle = (\sigma_\mu^\dagger)_{ab}|\beta_\mu\rangle. \tag{2.2}$$

Summation over repeated indices is implied and the four Pauli matrices are chosen as

$$\begin{aligned} \sigma_0 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & \sigma_1 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \sigma_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \sigma_3 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \end{aligned} \tag{2.3}$$

Note that the anti-symmetric Pauli matrix is σ_3 (rather than the more common choice σ_2), a choice also made in [25].

Proposition 2.2. *The basic two-qubit operations, $\sigma_\alpha \otimes \sigma_\beta$, act on the Bell states as a permutation (up to phase factors), and generate the symmetry group of the tetrahedron.*

Proof. From Eq. (2.2)

$$\sigma_\alpha \otimes \sigma_\beta |\beta_\mu\rangle = \frac{1}{\sqrt{2}} (\sigma_\alpha \sigma_\mu \sigma_\beta^\dagger)_{ab} |ab\rangle. \tag{2.4}$$

Since

$$\sigma_\mu \sigma_\nu = \begin{cases} i\epsilon_{\mu\nu k} \sigma_k, & \mu \neq \nu, k \in \{1, 2, 3\}; \\ \sigma_0, & \mu = \nu; \\ \sigma_\mu, & \nu = 0; \\ \sigma_\nu, & \mu = 0. \end{cases} \tag{2.5}$$

We see that $\sigma_\alpha \otimes \sigma_\beta$ just permutes the Bell states (up to phase factors). Since $\frac{1}{2}(1 + i\sigma_j) \otimes (1 + i\sigma_j)^\dagger$ interchange $|\beta_0\rangle \leftrightarrow |\beta_j\rangle$, they generate the permutation group of the four Bell states, S_4 . It is a fact that the tetrahedral group coincides with S_4 . \square

The Bell projections play a key role in what we do.

Proposition 2.3. *The Bell projection $P_\mu = |\beta_\mu\rangle\langle\beta_\mu|$ (no summation over μ , of course) have the form*

$$\begin{aligned} 4P_0 &= \sigma_0^{\otimes 2} + \sigma_1^{\otimes 2} + \sigma_2^{\otimes 2} - \sigma_3^{\otimes 2}, \\ 4P_1 &= \sigma_0^{\otimes 2} + \sigma_1^{\otimes 2} - \sigma_2^{\otimes 2} + \sigma_3^{\otimes 2}, \\ 4P_2 &= \sigma_0^{\otimes 2} - \sigma_1^{\otimes 2} + \sigma_2^{\otimes 2} + \sigma_3^{\otimes 2}, \\ 4P_3 &= \sigma_0^{\otimes 2} - \sigma_1^{\otimes 2} - \sigma_2^{\otimes 2} - \sigma_3^{\otimes 2}, \end{aligned} \tag{2.6}$$

where we denote

$$\sigma_\mu^{\otimes 2} = \sigma_\mu \otimes \sigma_\mu. \tag{2.7}$$

Proof. From Eq. (2.2) one finds (no summation over μ below)

$$\begin{aligned} 8P_\mu &= 4(\sigma_\mu)_{ab}(\sigma_\mu)_{dc}|a\rangle\langle c| \otimes |b\rangle\langle d| = (\sigma_\mu)_{ab}(\sigma_\mu)_{dc}(\sigma_\beta)_{ca}(\sigma_\alpha)_{db} \sigma_\beta \otimes \sigma_\alpha \\ &= \text{Tr} (\sigma_\beta \sigma_\mu \sigma_\alpha^\dagger \sigma_\mu) \sigma_\beta \otimes \sigma_\alpha. \end{aligned} \tag{2.8}$$

We used

$$2|a\rangle\langle c| = \text{Tr}(|a\rangle\langle c| \sigma_\beta) \sigma_\beta = (\sigma_\beta)_{ca} \sigma_\beta. \tag{2.9}$$

Since the Pauli matrices either commute or anti-commute, are either symmetric or antisymmetric, and are mutually orthogonal we have (no summation over μ here)

$$\text{Tr} (\sigma_\beta \sigma_\mu \sigma_\alpha^t \sigma_\mu) = \pm \text{Tr} (\sigma_\beta \sigma_\alpha^t) = \pm \text{Tr} (\sigma_\beta \sigma_\alpha) = \pm 2\delta_{\alpha,\beta} \tag{2.10}$$

Hence, only the diagonals survive in Eq. (2.8). \square

2.1. Teleportation

Bell states can be used to teleport [5] an unknown qubit. This is a consequence of the following teleportation lemma:⁴

Lemma 2.4. *Let $|\psi\rangle$ be a single qubit pure state. Then the following identity holds*

$$2|\psi\rangle \otimes |\beta_\mu\rangle = |\beta_\nu\rangle \otimes |\sigma_\mu^t \sigma_\nu \psi\rangle. \tag{2.11}$$

Proof. From Eq. (2.2):

$$\begin{aligned} 2|\psi\rangle \otimes |\beta_\mu\rangle &= \sqrt{2}\psi_c(\sigma_\mu)_{ab}|c\rangle \otimes |a\rangle \otimes |b\rangle = \psi_c(\sigma_\mu)_{ab}(\sigma_\nu^t)_{ca}|\beta_\nu\rangle \otimes |b\rangle = (\sigma_\mu^t \sigma_\nu \psi)_b |\beta_\nu\rangle \otimes |b\rangle \\ &= |\beta_\nu\rangle \otimes |\sigma_\mu^t \sigma_\nu \psi\rangle. \quad \square \end{aligned} \tag{2.12}$$

The identity has the following physical interpretation: The left-hand side describes the situation where Alice has the (unknown) qubit $|\psi\rangle$ and shares with Bob the Bell state $|\beta_\mu\rangle$. The right-hand side describes the superposition of the following situations: Alice pair of qubits is in one of the four Bell states while Bob’s qubit is a unitary transformation of $|\psi\rangle$. Alice can then measure in the Bell basis and tells Bob which Bell state she finds. Bob then performs the unitary operation $\sigma_\nu \sigma_\mu^t$ on his qubit to retrieve $|\psi\rangle$.

2.2. The CHSH Bell inequalities

The Bell states have the distinguished property that they give maximal violation of the CHSH Bell inequalities [13]. Bell inequalities [3] show that quantum mechanics cannot be simulated by classical probability theory [2,30,35,46,19]. This bit of theory follows simply from the formulas above for the Bell projections, as we now outline.

Let us denote by $a_{1,2}$ the result of Alice measurement of $\sigma_{1,2}$ and by $b_{+,-}$ the result of Bob measurement of $(\sigma_1 \pm \sigma_2)/\sqrt{2}$. All these measurements are dichotomic and yield only ± 1 . Any assignment of ± 1 to the corresponding four measurements yields

$$-2 \leq a_1(b_+ + b_-) + a_2(b_+ - b_-) \leq 2. \tag{2.13}$$

The same inequality must also hold on the average for any ensemble of classical systems. This is the CHSH Bell inequality [13,34,35].

Quantum mechanics is inconsistent with this inequality. To see this define the Bell operator [9] to be the observable corresponding to Eq. (2.13):

$$\begin{aligned} \mathbf{B} &= \sigma_1 \otimes \left(\frac{\sigma_1 + \sigma_2}{\sqrt{2}} + \frac{\sigma_1 - \sigma_2}{\sqrt{2}} \right) + \sigma_2 \otimes \left(\frac{\sigma_1 + \sigma_2}{\sqrt{2}} - \frac{\sigma_1 - \sigma_2}{\sqrt{2}} \right) = \sqrt{2}(\sigma_1^{\otimes 2} + \sigma_2^{\otimes 2}) \\ &= 2\sqrt{2}(P_0 - P_3). \end{aligned} \tag{2.14}$$

Clearly, $|\beta_0\rangle, |\beta_3\rangle$ are eigenstates of \mathbf{B} with eigenvalues $\pm 2\sqrt{2}$ and hence violate Eq. (2.13). The probabilistic aspect of quantum mechanics cannot be attributed to a classical probabilistic source that prepares the qubits of Alice and Bob.

⁴ The formula seems to be related to a formula in [53].

3. Separable states

In classical probability theory, random variables x and y are independent when their joint probability distribution is a product $P_A(x)P_B(y)$. Any joint probability distribution $P_{AB}(x,y)$ can be trivially written as a convex combination of product distributions:

$$P_{AB}(x,y) = \sum_{\alpha,\beta} P_{AB}(\alpha, \beta) \delta_{x,\alpha}\delta_{y,\beta}, \tag{3.1}$$

where $P_{AB}(\alpha, \beta)$ are thought of as weights and the two delta functions as probability measures.

This is not true in quantum mechanics [19]. A state ρ , a positive matrix with unit trace, is the analog of a probability measure. A state of the form $\rho_A \otimes \rho_B$ describes the situation where Alice's and Bob's qubits are uncorrelated. However, it is *not true* that all states can be written as convex combinations of uncorrelated states. The states that can be written in this way are called *separable* [50,25].

Definition 3.1. A (normalized) state ρ_s is separable if

$$\rho_s = \sum_{n=1}^N p_n \rho_A^{(n)} \otimes \rho_B^{(n)}, \tag{3.2}$$

with $p_n \geq 0$ probabilities and $\rho_{A,B}^{(n)}$ positive operators with normalized trace. A state $\rho \geq 0$ which is not separable is *entangled*.

Clearly, the unnormalized separable states make a convex cone contained in the cone of all positive (unnormalized) states.

Separable states can be interpreted as mixtures of uncorrelated states where Alice and Bob rely on a common probability distribution, p_n to create the mixture. This correlates Alice and Bob. Such correlation never violates Bell inequalities. For the CHSH this can be seen from the fact that for any product state

$$|\text{Tr}(\mathbf{B}\rho_A \otimes \rho_B)| = |a_1(b_+ + b_-) + a_2(b_+ - b_-)| \leq |b_+ + b_-| + |b_+ - b_-| \leq 2,$$

where now

$$|a_{1,2}| = |\text{Tr}(\sigma_{1,2}\rho_A)| \leq 1, \quad |b_{+,-}| = \left| \text{Tr} \left(\frac{\sigma_1 \pm \sigma_2}{\sqrt{2}} \rho_B \right) \right| \leq 1. \tag{3.3}$$

This result extends to separable states by convexity.

States that violate a Bell inequality are necessarily entangled. However, there are lots of entangled states that *do not* violate any CHSH inequality. (The equivalence classes of states that satisfy the CHSH inequality and their visualization is given in [1].)

There are no known general conclusive tests of separability. However, for two qubits the Peres–Horodecki partial transposition test [36,23] gives a simple spectral test of separability. To describe this test we first explain the notion of partial transposition for two qubits.

Any observable (Hermitian matrix) in the space of two qubits can be written as

$$A = A^{\mu\nu} \sigma_\mu \otimes \sigma_\nu, \quad A^{\mu\nu} \in \mathbb{R}. \tag{3.4}$$

For reasons that shall become clear later we call $A^{\mu\nu}$ the (contravariant) *Lorentz components* of A . The partial transpose of A , which we denote by A^P , is

$$A^P = A^{\mu\nu} \sigma_\mu \otimes \sigma_\nu^t = (A^P)^{\mu\nu} \sigma_\mu \otimes \sigma_\nu. \tag{3.5}$$

Observing that only σ_3 is anti-symmetric we see that the partial transpose, when expressed in terms of the Lorentz components, takes the form

$$(A^P)^{\mu\nu} = \begin{cases} A^{\mu\nu}, & \nu \neq 3; \\ -A^{\mu\nu}, & \nu = 3. \end{cases} \tag{3.6}$$

The Peres–Horodecki test is [36,23].



Fig. 3. A cone with opening angle θ is dual to the cone with opening angle $\pi-\theta$. The quadrant (left) is self-dual. The half-plane (right) is dual to the positive half-line. Here the usual scalar product of vectors corresponds to the trace in Eq. (4.1).

Theorem 3.2. A two qubit state $\rho \geq 0$ is separable iff $\rho^P \geq 0$.

Proof. The “only if” part is easy: If ρ is separable, it can be written as in Eq. (3.2). Since $\rho_B \geq 0$ implies that also $\rho_B^t \geq 0$, one has that ρ^P , being a convex combination of positive operators, is also positive. The “if” part requires more preparations. We shall give a simple geometric proof in Section 11. \square

4. Witnesses

Witnesses are observables which can give evidence that a state is entangled. For our present purposes it is convenient to slightly widen this notion and to allow for witnesses which are in a sense trivial. We therefore define the cone of *potential witnesses* as follows:

Definition 4.1. The dual cone⁵ to the cone of separable states shall be called the cone of *potential witnesses*. Explicitly, it is the collection of all observables W such that

$$\text{Tr}(W\rho_s) \geq 0, \tag{4.1}$$

for all separable states ρ_s . We shall call $-\text{Tr}(W\rho)$ the (*entanglement*) *evidence*.

A potential witness is called simply a witness iff there exist some (necessarily entangled) state ρ such that $\text{Tr}(W\rho_s) < 0$. The witness then gives conclusive evidence that ρ is entangled. In fact by standard duality arguments [40] the definition implies.

Proposition 4.2. Any entangled state, ρ , has a witness W giving positive evidence, i.e.

$$-\text{Tr}(W\rho) > 0. \tag{4.2}$$

The set of potential witnesses (unlike witnesses proper) is a convex set. A potential witness W may not give positive evidence for any state ρ . Clearly, this will be the case whenever $W \geq 0$. Thus the cone of potential witnesses contains the cone of states:

$$\text{Potential Witnesses} \supset \text{States} \supset \text{Separables}. \tag{4.3}$$

Observe that since $\rho = \mathbb{1}$ is clearly a separable (un-normalized) state it follows that any potential witness W has $\text{Tr} W \geq 0$. Moreover, the following holds:

Theorem 4.3. For any potential witness W , not identically zero:

$$\text{Tr} W > 0. \tag{4.4}$$

In particular, witnesses, like states, may be normalized to have unit trace.

Proof. Note that the elements $\langle \varphi \otimes \psi | W | \varphi \otimes \psi \rangle$ suffice to determine all other matrix elements of W . This may be verified by considering the case $\varphi \otimes \psi = (\varphi_1 + e^{i\alpha}\varphi_2) \otimes (\psi_1 + e^{i\beta}\psi_2)$ for all α 's and β 's. For any $W \neq 0$ one can therefore always find a normalized product state $|\varphi_0\rangle \otimes |\psi_0\rangle$ such that $\langle \varphi_0 \otimes \psi_0 | W | \varphi_0 \otimes \psi_0 \rangle > 0$. Complete this to an orthonormal product base $\{|\varphi_a\rangle \otimes |\psi_b\rangle\}_{a,b=0,1}$. Since

$$\text{Tr} W = \langle \varphi_a \otimes \psi_b | W | \varphi_a \otimes \psi_b \rangle, \tag{4.5}$$

(summation implied), has no negative terms one concludes the strict inequality. \square

⁵ The notion of dual cones is illustrated in Fig. 3.

It remains to demonstrate that there indeed are entangled states or, equivalently, that the inequality equation (4.3) is strict. An example for a witness that is not a positive operator is the swap, which exchanges the qubits of Alice and Bob:

$$S|\psi\rangle \otimes |\phi\rangle = |\phi\rangle \otimes |\psi\rangle. \tag{4.6}$$

Proposition 4.4. *The swap has the following properties:*

1. *S is positive on separable states.*
2. *$S = P_0 + P_1 + P_2 - P_3$ gives positive evidence that the singlet is entangled.*
3. *The swap is the partial transpose of a Bell projection: $S = 2P_0^p$.*

Proof. That S is positive on all pure product states follows from:

$${}_A\langle\psi| \otimes {}_B\langle\phi| S |\psi\rangle_A \otimes |\phi\rangle_B = \langle\psi|\phi\rangle_A \langle\phi|\psi\rangle_B = |\langle\psi|\phi\rangle|^2. \tag{4.7}$$

It is then positive on all separable states by convexity and so belongs to the cone of potential witnesses. This proves 1. Part 2 follows by noting that the Bell states are eigenvectors of the swap. Part 3 follows from the observation that swap can be written as $S = |ab\rangle\langle ba|$, while $P_0 = \frac{1}{2}|aa\rangle\langle bb|$. \square

It is, of course, not a coincidence that the swap is a witness of a Bell state. In Fig. 1 Bell states are represented by the (blue) dots at the vertices of the tetrahedron and the optimal witnesses by the red dots at the corners of the cube obtained by reflection about the three axes. We shall see in Corollary 7.2, that the swap is, in fact, an optimal witness.

5. Equivalence and local operations

We shall consider equivalence classes where ρ and ρ^M are considered equivalent provided

$$\rho \mapsto \rho^M = M\rho M^\dagger, \quad M = M_A \otimes M_B, \tag{5.1}$$

with $M_{A,B}$ taking values in the groups

$$SU(2) \subset SL(2, \mathbb{C}) \subset GL(2, \mathbb{C}). \tag{5.2}$$

The equivalence clearly preserves the positivity and the separability of states but, in general, not its normalization.

$M_{A,B} \in SL(2, \mathbb{C})$ will turn out to be our main tool and shall be designated by the acronym LSL for *local, special (-unit determinant) and linear*.

The linear maps in Eq. (5.1) with $M_{A,B} \in SL(2, \mathbb{C})$ or $GL(2, \mathbb{C})$ do not represent, in general, operations that Alice and Bob can perform on their qubits. Legitimate *quantum operation* are positivity preserving and trace non-increasing [35,34]. This means that M in Eq. (5.1) must satisfy $M^\dagger M \leq 1$. Quantum operation with $M^\dagger M < 1$ are interpreted as a generalized measurement, aka POVM [14,19,35,34,8].

When $M_{A,B} \in SL(2, \mathbb{C})$ or $GL(2, \mathbb{C})$, $M^\dagger M \not\leq 1$ so the linear map in Eq. (5.1) do not represent legitimate quantum operations. Nevertheless, with every such group element M we can associate the bona-fide POVM element

$$M \mapsto \frac{M}{\|M\|}. \tag{5.3}$$

The corresponding measurement filters [33,11] the state

$$\rho \mapsto \frac{M\rho M^\dagger}{\text{Tr}(M\rho M^\dagger)}. \tag{5.4}$$

Filtering wastes a fraction of the qubits, which Alice and Bob need to discard. Indeed, the filtration succeeds with probability

$$p(\rho) = \frac{\text{Tr}(M\rho M^\dagger)}{\|M\|^2} \leq 1. \tag{5.5}$$

(With $M_{A,B} \in SU(2)$ the “filtration” succeeds with probability one, but with $M_{A,B} \in SL(2, \mathbb{C}), GL(2, \mathbb{C})$ not.) Alice and Bob need to communicate over a classical channel, so they both keep only the qubits that pass the tests. This makes LSL a special case of SLOCC.

The equivalence classes introduced in Eq. (5.1) therefore admit the interpretation that two states are equivalent provided each can be filtered from the other and the filtration succeeds with finite probability. This imposes a restriction on what Alice and Bob are allowed to do. In particular, mixing is not an admissible operation. This is easily seen from the fact that M preserves the rank of ρ and so maps pure states to (unnormalized) pure states.

5.1. The equivalence classes of a single qubit

To appreciate the various notions of equivalence introduced above consider a single qubit. Any single qubit state ρ , can be identified with a (real) four-vector r_μ

$$\rho = r^\mu \sigma_\mu. \tag{5.6}$$

We shall refer to r^μ as the (contravariant) “Lorentz components” of ρ . States admit the following simple geometric characterization:

Lemma 5.1. *The four-vector r^μ represents an (un-normalized) state iff it lies in the forward light-cone. Pure states are light-like. Normalized states lie on the time slice $t = \frac{1}{2}$.*

Proof. This easily follows from

$$\det \rho = r^\mu r^\nu \eta_{\mu\nu}, \quad \text{Tr} \rho = 2r^0, \tag{5.7}$$

where η is the Minkowsky metric tensor, $\eta = \text{diag}(1, -1, -1, -1)$. Positivity $\rho > 0$ requires that both the trace and determinant are non-negative. The four-vector r^μ must then lie in the forward light cone. A pure state, being rank one, has $\det \rho = 0$ and is represented by a light-like vector. A normalized state has $\text{Tr} \rho = 2r^0 = 1$ and so lies on the fixed time-slice. \square

It follows from Eq. (5.7) that if $\rho^M = M\rho M^\dagger$, with $M \in SL(2, \mathbb{C})$ then the Lorentz component indeed transform like a vector under Lorentz transformation

$$(r^M)^\mu = (A_M)^\mu_\nu r^\nu, \tag{5.8}$$

where $A_M \in SO_+(1, 3)$ is an (orthochronous) Lorentz transformation. If $M \in SU(2)$ then it just rotates the spatial part of the four-vector.

It is instructive to compare the equivalence classes associated with normalized states of a single qubit with M taking values in the three groups $SU(2), SL(2, \mathbb{C}), GL(2, \mathbb{C})$, shown in Fig. 4.

- $SU(2)$ acts as spatial rotations and can be used to map any normalized state to the x - t -plane at time slice $t = \frac{1}{2}$.
- $SL(2, \mathbb{C})$ acts as Lorentz transformations and can be used to transform any time-like vector to the time-axis and any light-like vectors to any other light-like vector. This means that the LSL equivalence classes are represented by the semi-open interval $(0, \frac{1}{2}]$ and a point. It is natural to close the interval by gluing the point to the origin (since a light-like vector can be transformed to the origin of the time axis in the limit of infinite boosts). The $SL(2, \mathbb{C})$ and $SU(2)$ equivalence classes of *normalized* one qubit states are then in 1-1 correspondence.
- The $GL(2, \mathbb{C})$ equivalence classes, however, are represented by two points: One representing all pure states (light-like vectors) and one representing all mixed states.

For a normalized qubit the von Neumann entropy, $H(\rho) = -\text{Tr}(\rho \log_2 \rho)$, is uniquely determined by $\det \rho$. To see this express λ be the large eigenvalue of ρ , as $2\lambda = 1 + \sqrt{1 - 4 \det \rho}$. Then

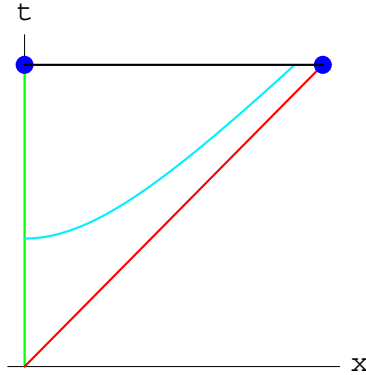


Fig. 4. The light cone is represented by the diagonal (red) line. The equivalence classes of the $SU(2)$ (normalized) states are represented by the horizontal (black) line at fixed time. The $GL(2, \mathbb{C})$ equivalence classes are the two (blue) dots. The dot on the time axis represents the equivalence class of mixed states and the other, on the light cone, the pure states. The $SL(2, \mathbb{C})$ equivalence classes are represented by the vertical green line. Light-like vectors can be brought to this line only through infinite boost. Points representing the $SU(2)$ and $SL(2, \mathbb{C})$ equivalence classes that lie on the same interval, $t^2 - x^2 = \text{const}$, (cyan) have identical entropies. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this paper.)

$$H(\rho) = -h(\lambda) - h(1 - \lambda), \quad h(\lambda) = \lambda \log_2 \lambda. \tag{5.9}$$

Since $\det \rho$ is preserved by $SL(2, \mathbb{C})$ we see that LSL preserves the information on the entropy of the state (provided it is not renormalized). $GL(2, \mathbb{C})$ on the other hand, does not distinguish between mixed states with different entropies.

5.2. Equivalence classes of two-qubit pure states

Two-qubit pure states are conveniently represented either in the computational basis or in the Bell basis:

$$|\psi\rangle = Y_{ab} |a\rangle \otimes |b\rangle = \zeta^\mu |\beta_\mu\rangle, \quad \sqrt{2} Y = \zeta^\mu \sigma_\mu. \tag{5.10}$$

Summation over repeated indices is implied; $a, b \in \{0, 1\}$ and $\mu \in \{0, 1, 2, 3\}$. The state is normalized if $\text{Tr}(YY^\dagger) = \zeta_\mu \zeta_\mu^* = 1$. This means that the pure states are described by the seven-sphere S^7 [55,32].

Local transformations take $|\psi\rangle$ to

$$M_A \otimes M_B |\psi\rangle = (M_A Y M_B^\dagger)_{ab} |a\rangle \otimes |b\rangle. \tag{5.11}$$

We see that $\det Y$ is invariant under the action of $M_{A,B} \in SL(2, \mathbb{C})$. As we shall see in the next section, $|\det Y|$ is a measure of the entanglement. This makes the entanglement an LSL invariant.

5.3. Entanglement distillation of pure states

The entanglement of a pure bi-partite normalized state is *defined* as the von Neumann entropy of either of its subsystems:

$$e(|\psi\rangle) = H(\rho_A) = H(\rho_B). \tag{5.12}$$

In the case at hand, where $|\psi\rangle$ is given by the matrix Y of Eq. (5.10)

$$\rho_A = Y Y^\dagger, \quad \rho_B = Y^\dagger Y. \tag{5.13}$$

It follows from Eq. (5.13) that

$$\det \rho_A = \det \rho_B = |\det Y|^2. \tag{5.14}$$

By Eq. (5.9) $\det \rho_A$ determines the entropy of Alice’s qubit. It follows that the measure of entanglement is uniquely determined by $\det Y$. Moreover, since $\det Y$ is invariant under LSL by Eq. (5.11), we see that LSL is a useful equivalence not just for describing the *notion* of entanglement, but also for describing its *measure*.

One must distinguish between the (mathematical) fact that the information on the measure of entanglement is preserved under LSL and the (physical) principle that local operations dissipate entanglement [38]. The difference comes from the way both treat the issue of normalization. An example, consider

$$|\psi_\theta\rangle = \cos \theta|00\rangle + \sin \theta|11\rangle, \quad 0 \leq \theta \leq \pi/4. \tag{5.15}$$

The LSL operation

$$M = \left(\sqrt{\tan \theta}|0\rangle\langle 0| + \sqrt{\cot \theta}|1\rangle\langle 1| \right) \otimes \mathbb{1} \tag{5.16}$$

filters from it the fully entangled unnormalized Bell state $\sqrt{2 \sin \theta \cos \theta}|\beta_0\rangle$. The information on the original measure of entanglement sits in the normalization. At the same time the corresponding quantum operation dissipates entanglement. By Eq. (5.5), the operation succeeds with probability

$$p(|\psi_\theta\rangle) = 2 \sin^2 \theta. \tag{5.17}$$

Using the fact $e(|\beta_0\rangle) = 1$ one ends up with less entanglement:

$$p(|\psi_\theta\rangle) = p(|\psi_\theta\rangle)e(|\beta_0\rangle) \leq e(|\psi_\theta\rangle), \tag{5.18}$$

in accordance with the principle that local operations dissipate entanglement, see Fig. 5.

6. Duality of states and observables

6.1. Contragradient actions

States ρ and observables W naturally live in dual spaces since pairing the two, $\text{Tr}(\rho W)$, gives a number. It is both natural and convenient to define the operations so that they act on states and witnesses in a way that respects their duality. Namely:

$$\begin{aligned} \rho \mapsto \rho^M &= M^\dagger \rho M, \\ W \mapsto W^M &= M^{-1} W (M^{-1})^\dagger. \end{aligned} \tag{6.1}$$

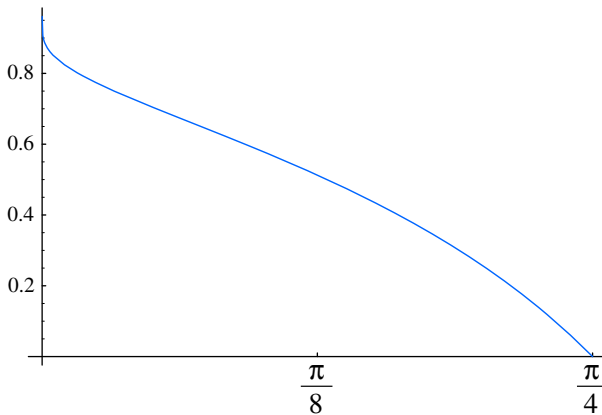


Fig. 5. The relative dissipation of the entanglement, $(e - p)/e$, for filtering Bell states from the states in Eq. (5.15) as a function of θ . The entanglement is e and the probability of filtering a Bell state is p . The graph expresses the inequality in Eq. (5.18).

If M is unitary, $M^{-1} = M^\dagger$, then states and observables transform the same way, but when M is only invertible, they do not. With this choice ρW undergoes a similarity transformation

$$\rho W \mapsto \rho^M (W)^M = M^\dagger (\rho W) (M)^{-1} \tag{6.2}$$

and $\text{Tr}(\rho W)$ is invariant.

When the local operations are taken from $SL(2, \mathbb{C})$, there is a map, the tilde map, that takes observables to states and vice versa. By this we mean that if A transforms as a state then \tilde{A} transforms as an observable, i.e.

$$(M^\dagger \tilde{A} M) = M^{-1} \tilde{A} (M^{-1})^\dagger. \tag{6.3}$$

For a single qubit the tilde map is given by

$$\tilde{A} = \sigma_3 A^\dagger \sigma_3 \tag{6.4}$$

and for a pair of qubits by

$$\tilde{A} = (\sigma_3 \otimes \sigma_3) A^\dagger (\sigma_3 \otimes \sigma_3). \tag{6.5}$$

That the tilde map indeed satisfies Eq. (6.3) is a property of $SL(2, \mathbb{C})$. It follows from the identity

$$\sigma_3 M^\dagger \sigma_3 = M^{-1}, \quad M \in SL(2, \mathbb{C}). \tag{6.6}$$

The tilde operation acts on the Pauli spin matrices as “spin-flip”, reversing the spatial component⁶

$$\tilde{\sigma}_\mu = \sigma_3 \sigma_\mu^\dagger \sigma_3 = \sigma^\mu. \tag{6.7}$$

(Indices are raised and lowered according to the Minkowsky metric tensor η). It follows that

$$\text{Tr}(\sigma_\mu \tilde{\sigma}_\nu) = 2\eta_{\mu\nu}. \tag{6.8}$$

If we represent single qubit states and observables by contravariant components of four-vectors

$$\rho = r^\mu \sigma_\mu, \quad W = w^\mu \tilde{\sigma}_\mu, \tag{6.9}$$

the invariance of $\text{Tr}(\rho W)$ implies that r^μ and w^μ transform under the same Lorentz transformation:

$$\text{Tr}(\rho W) = 2r^\mu w^\nu \eta_{\mu\nu}. \tag{6.10}$$

This carries over to two qubits where states and witnesses are represented by contravariant tensors

$$\rho = r^{\mu\nu} \sigma_\mu \otimes \sigma_\nu, \quad W = W^{\mu\nu} \tilde{\sigma}_\mu \otimes \tilde{\sigma}_\nu, \tag{6.11}$$

and now the Lorentz scalar is

$$\text{Tr}(\rho W) = 4r^{\mu\nu} W_{\mu\nu}. \tag{6.12}$$

6.2. Self-duals and anti-self-duals

We shall say that W_e is self-dual if

$$W_e = \tilde{W}_e. \tag{6.13}$$

For a single qubit self-duality means that the state is fully mixed. For two qubits, it readily follows from Eq. (6.7) that the matrix of Lorentz components of W_e has the form

$$W_e = \begin{pmatrix} W_{00} & 0 & 0 & 0 \\ 0 & W_{11} & W_{12} & W_{13} \\ 0 & W_{21} & W_{22} & W_{23} \\ 0 & W_{31} & W_{32} & W_{33} \end{pmatrix}. \tag{6.14}$$

⁶ The notation used in high energy physics [37] is bar rather than tilde. We use tilde to be consistent with Wootters [51].

The space of self-duals is then evidently 10 dimensional. Self-dual states are states having fully mixed subsystems. Self-dual observables are time-reversal invariant.

Since $SU(2)$ act on the (spatial) of the Pauli matrices like a rotation, the singular value decomposition implies that

Proposition 6.1. *Every self-dual W_e can be brought to a canonical form*

$$W_e \rightarrow w_\mu \sigma_\mu^{\otimes 2} = \omega_\mu P_\mu \tag{6.15}$$

by a pair of $SU(2)$ transformation, where $w_0 = W_{00}$ and the spatial components, w_j are the singular values of the 3×3 sub-matrix of W_e (up to sign⁷). The ω_μ and w_μ are related by the linear transformation of Eq. (2.6)

$$\begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{pmatrix}. \tag{6.16}$$

In particular, the ω_μ are all real.

The space of (not necessarily hermitian) anti-self-dual operators may be identified with the Lie algebra of $SL(2, \mathbb{C}) \otimes SL(2, \mathbb{C})$. Indeed by Eq. (6.6)

$$\tilde{M} = M^{-1}, \quad \forall M \in SL(2, \mathbb{C}) \otimes SL(2, \mathbb{C}) \tag{6.17}$$

from which follows

$$\delta \tilde{M} = -M^{-1} (\delta M) M^{-1}. \tag{6.18}$$

The Lie algebra is the variation at the identity where $\delta \tilde{M} = -\delta M$, i.e. the Lie algebra is anti-self-dual. Since the linear space of anti-self-dual operators is 6-complex-dimensional (spanned by $\sigma_i \otimes 1, 1 \otimes \sigma_i; i = 1, 2, 3$) it must coincide with the whole Lie algebra.

6.3. LSL invariants

Since \tilde{A} transform contragradiently to A , the product $\tilde{A}A$ undergoes a similarity transformation by Eq. (6.2). This allows us to associate spectral invariants with the LSL action:

Lemma 6.2. *For any (n -qubit) observable, the spectrum of $\tilde{A}A$ and $\det A$ are LSL invariants.*

To get a feeling for the invariants consider first the case of a single qubit state $\rho = r^\mu \sigma_\mu$. In this case there is just a single invariant

$$\tilde{\rho} \rho = (r_\mu r^\mu) \mathbb{1} = (\det \rho) \mathbb{1}. \tag{6.19}$$

By Eq. (5.9) the determinant encodes the information on the entropy of the (normalized) state and vanishes for pure states.

Multi-qubits observables of the form $\rho = \rho_A \otimes \rho_B$ then have as invariant $\det(\rho_A) \det(\rho_B)$. In particular, it follows that

$$\tilde{\rho} \rho = 0, \tag{6.20}$$

whenever either ρ_A or ρ_B is a pure state.

In the case of two qubits, $\text{spec}(\tilde{A}A)$ gives four LSL-invariants. The invariant $\det A$ is closely related to them, since

$$\det(\tilde{A}A) = (\det A) (\det \tilde{A}) = (\det A)^2. \tag{6.21}$$

Thus the only additional information supplied by $\det A$ is its sign.

⁷ Singular value decomposition requires $O(3)$ while we use only $SO(3)$.

In the particular case where A is a state we trivially have $\det A \geq 0$. As $\tilde{\rho}\rho$ is readily seen to be similar to the positive operator

$$\sqrt{\tilde{\rho}} \tilde{\rho} \sqrt{\tilde{\rho}}, \tag{6.22}$$

one evidently has in this case

Lemma 6.3 (Wootters [51]). *When $\rho > 0$ the eigenvalues of $\tilde{\rho}\rho$ are all positive.*

We define the LSL invariant spectrum of state ρ as the positive roots of the eigenvalues of $\tilde{\rho}\rho$.

Since a witness W is, in general, not positive, it is not a priori clear that eigenvalues of $\tilde{W}W$ are positive. In fact, for a general observable A , the spectrum of $\tilde{A}A$ need not even be real. We shall see, in the next section, that for witnesses the eigenvalues of $\tilde{W}W$ are still positive. Moreover, as we shall see, there is a natural way to choose signs for the roots of these eigenvalues in a way that is consistent with the invariance of $\det W$. This will allow defining the LSL invariant spectrum of W in a way that amalgamate the two invariants of Lemma 6.2.

7. Canonical forms as optimizers

We want to extend the notion of LSL invariant spectrum to witnesses. Since witnesses are, in general, not positive, the argument leading to Lemma 6.3 does not apply. However, as we shall see, the LSL invariant spectrum $\{\omega_\mu\}$ is still well defined and real. In fact the following key result holds:

Theorem 7.1. *Any observable W in the interior of the cone of potential witnesses is LSL equivalent to a witness of canonical form*

$$W \mapsto \omega_\mu P_\mu, \tag{7.1}$$

where P_μ are the Bell projections, $\omega_\mu \in \mathbb{R}$, and ω_μ^2 are the eigenvalues of $\tilde{W}W$. The representation (7.1) is unique, up to permutations of the ω_μ 's. This generate the tetrahedral group manifest in Fig. 1. A unique representation is obtained by imposing the canonical order

$$\omega_0 \geq \omega_1 \geq \omega_2 \geq |\omega_3|. \tag{7.2}$$

In particular, at most one LSL-eigenvalue, the one with smallest magnitude, is negative.

The upshot of this theorem is that the LSL equivalence classes of the 16-dimensional cone of potential witnesses, and therefore also the cone of (un-normalized) states, can be represented by points in \mathbb{R}^4 .

The proof of this theorem depends on a variational principle. Specifically on finding a witness that maximizes the entanglement evidence, in the sense of Definition 4.1. This point of view leads to our second key result:

Theorem 7.2. *Let W and ρ be in the interior of the cone of potential witnesses, and let $W_e = \omega_\mu P_\mu$ and $\rho_e = \rho_\mu P_\mu$ be their associated canonical forms. Then*

$$\min_M \left\{ \text{Tr}(W^M \rho) \right\} = \text{Tr}(W_e \rho_e) = \sum_\mu \rho_\mu \omega_\mu, \tag{7.3}$$

where ρ_μ are chosen in canonical order, Eq. (7.2), while ω_μ are chosen with the anti-canonical order

$$\omega_0 \leq \omega_1 \leq \omega_2 \leq \omega_3. \tag{7.4}$$

In particular, taking $\rho = 1$, we see that the LSL map $W \mapsto \omega_\mu P_\mu$ is trace decreasing.

Corollary 7.3. *It follows that to test whether a state is entangled it is enough to test its canonical representer against canonical witnesses.*

The proofs of both theorems are given in the following subsections.

7.1. Existence of the optimizer

Consider the stationary points of the function $M \mapsto \text{Tr}(\rho W^M)$ where $M = M_A \otimes M_B$. For $M_{A,B} \in SU(2)$, this function must have (finite) maximum and minimum⁸ since $SU(2)$ is compact. However, in the case that $M_{A,B} \in SL(2, \mathbb{C})$, which is not compact, there may be no stationary point for any finite M . The existence of a minimum is guaranteed by the following lemma.

Lemma 7.4. *Suppose ρ and W both lie in the interior of the cone of potential witnesses, i.e. satisfying a strict inequality in (4.1). Then, the function $\text{Tr}(\rho W^M)$, diverges to $+\infty$ as either $M_A \in SL(2, \mathbb{C})$ or $M_B \in SL(2, \mathbb{C})$ go to infinity. In particular, it has a finite minimizer.*

The lemma may be written in a more symmetric form (under $\rho \leftrightarrow W$) by noting

$$\text{Tr}(\rho^M W^N) = \text{Tr}(\rho W^{(M^{-1})^\dagger N}). \tag{7.5}$$

Sketch of the proof. The spectrum of any $M_A \in SL(2, \mathbb{C})$ is of the form $\{\lambda, 1/\lambda\}$. The element is large when $|\lambda|$ is large. It can then be approximated by a rank one operator (corresponding to the large eigenvalue) $M_A \simeq \lambda P$, with P a one-dimensional projection. Thus $M = M_A \otimes M_B \simeq \lambda P \otimes M_B$ is essentially supported on a $1 \otimes 2$ -dimensional subspace of the full $2 \otimes 2$ space. As a $1 \otimes 2$ space cannot support any entanglement, the corresponding expectation $\text{Tr}(\rho W^M) \simeq |\lambda|^2 \text{Tr}(\rho W^{P \otimes M_B})$ must be positive. As it is multiplied by $|\lambda|^2$ it actually diverge to $+\infty$ with λ . \square

An alternative proof of Lemma 7.4 and a generalization of it which applies to witnesses on the boundary are described in Appendix A.

7.2. Characterization of the optimizer

In the previous section, we have seen that $\text{Tr}(\rho W^M)$ has a minimizer. Once its existence is guaranteed, one may use standard variational procedure to characterize it. As we shall show whenever ρ is of the canonical form the minimizer – the optimal witness, is also of the form $\omega_\mu P_\mu$.

Note that the Bell projections are self-dual, $P_\mu = \tilde{P}_\mu$. We start by showing that the stationary points of $\text{Tr}(\rho W^M)$ are self-dual.

Lemma 7.5. *The stationary points of the function $\text{Tr}(\rho W^M)$, where $M = M_A \otimes M_B$ with $M_{A,B} \in SL(2, \mathbb{C})$ are the self-dual points, i.e.*

$$\widetilde{\rho W^M} = \rho W^M. \tag{7.6}$$

Proof. Suppose $\text{Tr}(\rho W^M)$ is stationary at the identity $M = I$ then for any small LSL-variation $M = I + \delta M$ we must have

$$\begin{aligned} 0 &= \delta \text{Tr}(\rho W^M) = \delta \text{Tr}(\rho M^{-1} W M^{-1 \dagger}) = \text{Tr}(\rho(-\delta M)W + \rho W(-\delta M^\dagger)) \\ &= -\text{Tr}(W \rho \delta M) - \text{Tr}(W \rho \delta M)^* = -2\text{Re Tr}(W \rho \delta M), \end{aligned} \tag{7.7}$$

where we used the fact that ρ, W are hermitian. Recall that by Eq. (6.17) the Lie algebra of LSL consists of complex matrices satisfying $\widetilde{\delta M} = -\delta M$. Stationarity requires $W \rho$ to be in the space orthogonal to these which is the space of self-duals $W \rho = \widetilde{W \rho}$. Formally this follows by using the identity $\text{Tr}(\widetilde{A B}) = \text{Tr}(A B)$ to write

$$0 = \delta \text{Tr}(\rho W^M) = -\text{Re Tr}(\delta M (W \rho - \widetilde{W \rho})). \tag{7.8}$$

⁸ In fact by Morse theory it must have at least one maximum, one minimum and two saddles.

As both δM and $W\rho - \widetilde{W}\rho$ are anti-self-dual, the trace of their product vanishes for arbitrary (complex) anti self-dual δM if and only if $W\rho = \widetilde{W}\rho$. A stationary point at arbitrary M similarly lead to (7.6). \square

It follows that any strict potential witness W is LSL-equivalent to a self-dual one. To see this take $\rho = 1$. Lemma 7.4 then guarantees that $\text{Tr}(W^M)$ has a minimum, and Lemma 7.5 tells us that the minimizer W^M is self-dual. Moreover, by applying Proposition 6.1 it follows that W can be brought to a canonical form, Eq. (7.1). The lemma below gives a direct proof of this fact without relying on the singular value decomposition used in Proposition 6.1.

Lemma 7.6. *Suppose the state ρ is self-dual, then $\text{Tr}(\rho W^M)$ has its stationary points where $[\rho^2, W^M] = 0$. In particular if ρ is in canonical form Eq. (7.1), then (at least in the generic non-degenerate case) so is the minimizer W^M . In the case of degenerate ρ^2 the minimizer W^M is not unique but may still be chosen as canonical.*

Proof. Combining $\rho = \tilde{\rho}$ with the minimizer condition (7.6) gives

$$(\rho W^M) = (\rho \widetilde{W^M}) = (\widetilde{W^M}) \tilde{\rho} = (\widetilde{W^M}) \rho, \tag{7.9}$$

and similarly

$$(W^M \rho) = (W^M \widetilde{\rho}) = \tilde{\rho} (\widetilde{W^M}) = \rho (\widetilde{W^M}). \tag{7.10}$$

Combining the two gives $\rho^2 W^M = W^M \rho^2$. Thus the Bell basis which diagonalize ρ must do the same for W^M , unless ρ^2 happens to be degenerate. In the special case of degenerate ρ^2 one may find a Bell-diagonalized minimizer W^M by considering first a small degeneracy breaking perturbation of ρ . \square

7.3. Proofs of the two theorems

Proof of Theorem 7.1. Choosing some generic ρ of the canonical form (7.1) and arbitrary W , we are guaranteed by Lemma 7.4 that $\text{Tr}(\rho W^M)$ has a minimum. Lemma 7.6 then tells us that the minimizer W^M is also of the canonical form $\omega_\mu P_\mu$. The four eigenvalues ω_μ can be permuted arbitrarily by Proposition 2.2.

The LSL invariance of

$$\text{Spec}(\widetilde{W}W) = \{\omega_\mu^2\} \tag{7.11}$$

determines ω_μ up to sign. To determine the signs we shall show that at most one LSL-eigenvalue is negative. To this end, note first that from any pair of the Bell states, one may construct a separable state $|\beta_\mu\rangle + e^{i\varphi}|\beta_\nu\rangle$ (actually $e^{i\varphi} = 1$ or i). For example

$$|\beta_0\rangle + |\beta_1\rangle = \sqrt{2}|00\rangle, \quad |\beta_2\rangle + i|\beta_3\rangle = \sqrt{2}|01\rangle, \text{ etc.} \tag{7.12}$$

(Since local unitaries can permute Bell states, similar relations must hold for all other Bell pairs.) With W in canonical form we then have by Eq. (4.1) that

$$0 \leq \langle \beta_\mu + e^{i\varphi}\beta_\nu | W^M | \beta_\mu + e^{i\varphi}\beta_\nu \rangle = (\omega_\mu + \omega_\nu), \quad \mu \neq \nu. \tag{7.13}$$

This implies that at most one of the eigenvalues is negative, and moreover, it must be the one of smallest absolute value. The LSL-invariance of $\det(W)$ then fixes the signs of all the ω_μ uniquely. The proof is complete. \square

Proof of Theorem 7.2. Given W and ρ Theorem 7.1 tells us that that $\rho^N = \rho_e = \rho_\mu P_\mu$ for some $N \in SL(2, \mathbb{C}) \otimes SL(2, \mathbb{C})$. We therefore have

$$\text{Tr}(\rho W) = \text{Tr}(\rho_e^{N-1} W) = \text{Tr}(\rho_e W^N) \geq \min_M \{ \text{Tr}(\rho_e W^M) \}. \tag{7.14}$$

By Lemma 7.6 we know that $\text{Tr}(\rho_e W^M)$ is stationary whenever $W^M = \omega_\mu P_\mu$. The minimum clearly corresponds to requiring Eqs. (7.2) and (7.4). \square

7.4. The boundary of the cone of witnesses

Theorem 7.1 applies only to observables W in the interior of the cone of potential witnesses. It can be extended to the boundary, provided the notion of LSL-transformations is appropriately modified. We shall say that observable B is obtained by a generalized LSL-transformation from observable A iff it is in the closure of the equivalence class of A ,⁹ i.e. iff there exist a series $\{M_i\}_{i=1}^\infty \subset SL(2, \mathbb{C}) \otimes SL(2, \mathbb{C})$ such that $A^{M_i} \rightarrow B$. Theorems 7.1 and 7.2 then hold in this generalized sense for any potential witness (with \min_M replaced by \inf_M). The proof follows very similar lines to the proofs given above. The only major change is replacing Lemma 7.4 by a generalization of it described in Appendix A.

8. Classification: a Lorentzian picture

8.1. Geometric characterization of witnesses

The matrix of Lorentz components $W_{\mu\nu}$ of a potential witness W , Eq. (6.11), allows for a simple geometric characterization of potential witnesses. By definition, a potential witness has positive expectation for product states:

$$0 \leq \text{Tr} (W \rho_A \otimes \rho_B) = 4W_{\mu\nu} (\rho_A)^\mu (\rho_B)^\nu. \tag{8.1}$$

Since the four-vectors $(\rho_{A,B})_\mu$ can lie anywhere in the forward light cone (by Lemma 5.1), we learn that the matrix W maps the forward light cone into itself. Points that lie in the interior of the cone of potential witnesses satisfy a strict inequality in Eq. (8.1). The map W then sends the forward light cone into its (timelike) interior.

8.2. Lorentz singular values

By Eq. (5.8) LSL acts on the Lorentz components of a two-qubit observable W by a pair of Lorentz transformations

$$W^{A \otimes B} = A_A W A_B^t, \tag{8.2}$$

where $A_{A,B} \in SO_+(1, 3)$ are two 4×4 Lorentz transformation matrices.

From Eq. (2.6) it follows that if W is in canonical form then

$$W = \omega_\mu P_\mu = w_\mu \sigma_\mu^{\otimes 2}, \tag{8.3}$$

so that the Lorentz matrix W is diagonal. We shall refer to w_μ as the **canonical coordinates** of W , and to ω_μ as the **spectral coordinates**. The ω_μ and w_μ coordinates are related by Eq. (6.16).

Thus when viewed in terms of Lorentzian components, bringing W to its canonical form consists of diagonalizing the associated tensor $W_{\mu\nu}$ by a pair of Lorentz transformations. This is reminiscent of the notion of the singular decomposition of a matrix (which is defined in the same way with the Lorentz transformation replaced by orthogonal matrices).

For a matrix M its singular values are the (positive) roots of the matrix $M^t M$. The Lorentzian analog of $M^t M$ turns out to be the matrix $W^{j\mu} W_{i\nu}$. It is convenient to write it as $W^\star W$ where the ‘Lorentz conjugated matrix’ is defined by¹⁰

$$W^\star = \eta W^t \eta. \tag{8.4}$$

One readily verifies that componentwise

⁹ This is not an equivalence relation as generalized transformations need not be invertible.

¹⁰ The \star duality, conforms with the Lorentz scalar product, $v \cdot (Wu) = (W^\star v) \cdot u$. It is distinct from the \sim duality of the previous section.

$$(W^\star)_{\mu\nu} = W^{\nu\mu}. \tag{8.5}$$

Since Lorentz transformations leave the Minkowsky metric invariant, $A^t \eta A = \eta$, one has

$$A^\star = A^{-1}. \tag{8.6}$$

It then follows that under (8.2) $W^\star W$ undergoes a similarity transformation

$$W^\star W \rightarrow (A_M W A_N^t)^\star (A_M W A_N^t) = (A_N^t)^{-1} (W^\star W) A_N^t, \tag{8.7}$$

and similarly for $W W^\star$. The spectra of $W^\star W$ and $W W^\star$ are therefore LSL invariant.

The LSL invariance of the spectrum of $W W^\star$ does not depend on W being a witness. In general, this spectrum is complex. For matrices that lie in the cone of witnesses one has, by Eq. (8.3), that the eigenvalues of $W W^\star$ are w_μ^2 and are positive (or zero). In this case, in analogy with the notion of singular values, one may define the Lorentz singular values as $|w_\mu|$.

Remark 8.1. Diagonal Lorentz transformations in $O(1,3)$ with ± 1 on the diagonal, bring any diagonal W to a positive diagonal form. However, we are allowed only proper orthochronous Lorentz transformations, $SO_+(1,3)$. Thus the canonical coordinates w_μ defined via Eq. (8.3) may differ in signs from the (positive) Lorentz singular values.

8.3. Tetrahedral symmetry and fundamental domains

The tetrahedral group acts on the coordinates ω_μ as permutations. In terms of the coordinates w_μ this group acts as permutations and sign flips of the three ‘spatial’ coordinates w_j which leave $\text{sgn}(w_1 w_2 w_3)$ invariant. To see this note first that the relation $4w_0 = \omega_0 + \omega_1 + \omega_2 + \omega_3 > 0$ shows that w_0 is independent of the ordering of ω_μ . Hence, the tetrahedral group acts only on the spatial components w_j . For proper Lorentz transformations $\det(W) = w_0 w_1 w_2 w_3$ cannot change sign. In cases when $\det(W) > 0$ the canonical coordinates may be taken as equal to the Lorentz singular values. If $\det(W) < 0$ then at least one of the canonical coordinates (which we will usually take to be the one having least absolute value) must be chosen as negative. The tetrahedral symmetry allows one to impose w_μ to be in the *fundamental domain*

$$w_1 \geq w_2 \geq |w_3|, \tag{8.8}$$

which is equivalent to Eq. (7.2). The *antipodal fundamental domain*

$$-w_1 \geq -w_2 \geq |w_3| \tag{8.9}$$

is equivalent to the anti-canonical ordering of Eq. (7.4).

8.4. Classification of potential witnesses

Symmetric matrices that map the forward light-cone into itself may be interpreted in general relativity as energy–momentum tensors that satisfy the ‘‘dominant energy condition’’. Their classification¹¹ is given in pp. 89–90 in [17]. We need a generalization of this classification to non-symmetric matrices¹² where we are allowed to use a pair of Lorentz transformations as in Eq. (8.2). The classification is given in [48] and is based on [15]:

Theorem 8.2. *Let W be a 4×4 matrix that maps the forward light-cone into itself. Fix arbitrary $\kappa > 0$. Then there is a pair of Lorentz transformations A_A, A_B such that $A_A W A_B$ is of one of the four canonical forms, unique subject to Eq. (8.8):*

- *The ordinary diagonal form*

¹¹ Landau and Lifshitz, p. 274 in [27], gives a partial classification.

¹² By (8.4) $W^\star = W$ means $W \eta$ is symmetric.

$$\begin{pmatrix} w_0 & 0 & 0 & 0 \\ 0 & w_1 & 0 & 0 \\ 0 & 0 & w_2 & 0 \\ 0 & 0 & 0 & w_3 \end{pmatrix}, \tag{8.10}$$

associated with the cone in four dimensions with a cross-section that is a three-dimensional cube:

$$w_0 \geq |w_j|. \tag{8.11}$$

- The first extraordinary form

$$\begin{pmatrix} w_0 + \kappa & -\kappa & 0 & 0 \\ \kappa & w_1 - \kappa & 0 & 0 \\ 0 & 0 & w_2 & 0 \\ 0 & 0 & 0 & w_3 \end{pmatrix}, \tag{8.12}$$

associated with the boundary of the cone

$$w_0 = w_1 \geq |w_{2,3}|. \tag{8.13}$$

- The second extraordinary form

$$\begin{pmatrix} \kappa & \kappa & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{8.14}$$

associated with the apex of the cone $w_\mu = 0$.

- The third extraordinary form

$$\begin{pmatrix} \kappa & 0 & 0 & 0 \\ \kappa & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{8.15}$$

also associated with the apex of the cone $w_\mu = 0$.

w_{μ} the “Lorentz singular values”, are roots of the eigenvalues of W^*W .

The proof of this theorem is given in [Appendix B](#).

9. The geometry of witnesses and states

We have seen that the LSL equivalence classes of witnesses, states and separable states are represented by nested cones in four dimensions. In this section we give a geometric description of these cones.

9.1. The geometry of ordinary witnesses

The Lorentz tensor associated with the witness

$$W_e = w_\mu \sigma_\mu^{\otimes 2} \tag{9.1}$$

maps the light cone into itself iff $w_0 \geq |w_j|$. The LSL equivalence classes of the (ordinary) potential witnesses are therefore characterized geometrically by the cone in four dimensions:

$$w_0 \geq |w_1|, |w_2|, |w_3|, \tag{9.2}$$

whose cross-section is the cube.

By [Theorem 7.2](#) the canonical representative of a witness also minimizes $\text{Tr}(W^M)$. Thus the representatives of normalized witnesses have $w_0 \leq \frac{1}{4}$ giving a capped cone. All points in the capped cone are relevant since given $W_e \neq 0$ with $\text{Tr } W_e < 1$ one easily finds M which makes $\text{Tr}(W_e^M)$ as large as one wants.

Four corners of the cube at the cap of the cone, making the vertices of a tetrahedron, represent the four Bell states P_μ . The four remaining corners, also making a tetrahedron, describe bona-fide Bell witnesses, all equivalent to the swap $S = \frac{1}{2} \sum \sigma_\mu^{\otimes 2}$.

9.2. The geometry of the ordinary separable states

The duality between separable states and potential witnesses in 16 dimensions translates to a duality between the cones of the corresponding equivalence classes in four dimensions. This follows from [Corollary 7.3](#) which says that the corresponding cones in \mathbb{R}^4 , defined by $\rho_\mu \omega_\mu \geq 0$ are also dual cones. The identity $\rho_\mu \omega_\mu = 4r_\mu w_\mu$ allows writing this in terms of canonical coordinates as $r_\mu w_\mu \geq 0$. Since the dual of the cube is the octahedron, the LSL equivalence classes of the separable states are represented by a cone whose cross-section is an octahedron.

Algebraically, the separable states are described by the eight extremal inequalities

$$\frac{1}{4} \geq r_0 \geq w_1 r_1 + w_2 r_2 + w_3 r_3, \quad w_i = \pm 1 \tag{9.3}$$

associated with the eight witnesses at the corners of the cube, making up an octahedral cone.

A different way [\[28\]](#) to see that the separable states are represented by the octahedron relies on considering explicitly the six operators corresponding to the vertices of the octahedron:

$$8S_{j\pm} = (\sigma_0 + \sigma_j) \otimes (\sigma_0 \pm \sigma_j) + (\sigma_0 - \sigma_j) \otimes (\sigma_0 \mp \sigma_j) = 2(\sigma_0^{\otimes 2} \pm \sigma_j^{\otimes 2}) \tag{9.4}$$

and $j = 1, 2, 3$. The middle expression shows that all six vertices are separable states. The right-hand side shows that they all are equal mixtures of any two Bell states.

9.3. The geometry of all ordinary states

Let ρ_e be a canonical representer corresponding to the state ρ , i.e.

$$\rho_e = r_\mu \sigma_\mu^{\otimes 2} = \rho_\mu P_\mu. \tag{9.5}$$

Since $\rho \geq 0$, the LSL equivalence classes are represented by the positive quadrant, $\rho_\mu \geq 0$, in four dimensions. This is evidently a cone whose cross-section is the tetrahedron.

In terms of the r coordinates the cone of all states is described by four out of the eight inequalities equation [\(9.3\)](#), specifically those corresponding to $w_1 w_2 w_3 = -1$.

The LSL equivalence classes corresponding to normalized states form a four-dimensional capped cone with

$$\sum \rho_\mu \leq 1. \tag{9.6}$$

The cap of the cone is the three-dimensional tetrahedron, and represents the $SU(2)$ equivalence classes of states with fully mixed subsystems.

The four vertices of the tetrahedron at the cap of the cone are identified with the four Bell states P_μ of Eq. [\(2.6\)](#) and represent a single equivalence class as the tetrahedral symmetry can interchange any of them, by [Proposition 2.2](#). The ρ_μ coordinate lines represent the (equivalence classes) of entangled pure states discussed in [Section 5.2](#).

The apex of the cone at the origin formally corresponds to the states where $\tilde{\rho} = 0$ which, by Eq. [\(6.20\)](#), occurs when at least one of the subsystems is pure, as in Eq. [\(1.1\)](#).

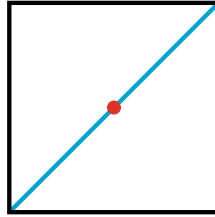


Fig. 6. The figure represents the extraordinary canonical forms associated with the boundary of the cube, Eq. (9.8) with $\kappa \neq 0$. The extraordinary separable states are represented by the red dot and the extraordinary entangled states by the cyan diagonal. The square represents extraordinary witnesses. The extraordinary canonical forms are inequivalent to the ordinary ones (corresponding to $\kappa = 0$) cohabiting the same set of points. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this paper.)

Any point in the cone of states can be expressed as a (sub) convex combination of its vertices representing the four Bell states.¹³

Corollary 9.1. *Any mixed two qubit state can be expressed as a convex combination of four pure states, each equivalent to a Bell state by the same LSL-transformation.*

The fundamental domain of normalized states is most simply described in terms of its spectral coordinates ρ_μ as

$$\rho_0 \geq \rho_1 \geq \rho_2 \geq \rho_3 \geq 0, \quad \sum \rho_\mu \leq 1$$

or, equivalently, by

$$\frac{1}{4} \geq r_0 \geq r_1 + r_2 + r_3, \quad r_1 \geq r_2 \geq |r_3|. \tag{9.7}$$

9.4. *The geometry of the boundary*

The boundary of the cone of potential witnesses is subtle. Observables inside the cone are guaranteed to have a finite LSL transformation that brings them to canonical form. However, as one approaches the boundary, it may happen that the required LSL transformation may or may not have a limit. If it does, the state/witness belongs to an ordinary class, if it does not, it belongs to an extraordinary LSL equivalence class. Both classes, though LSL inequivalent, have identical invariant spectra and Lorentz singular values and therefore are represented by the same point in four dimensions. This makes the set of LSL equivalence classes' non-Hausdorff.

The first extraordinary family, Eq. (8.12) of Theorem 8.2, with $w_1 = w_0$ and $w_2 + w_3 \neq 0$ describes observables with a negative eigenvalue which therefore are witnesses rather than states. When $w_2 = -w_3$ it describes the extraordinary family of a mixture of two Bell states and a pure product state

$$(p_0 P_0 + p_1 P_1) + \kappa(\sigma_0 + \sigma_1) \otimes (\sigma_0 - \sigma_1) \tag{9.8}$$

p_0, p_1 probabilities: $p_0 + p_1 \leq 1$ and $p_0, p_1 \geq 0$. For definiteness one may fix, e.g. $\kappa = 1$. The Lorentz singular values are seen to be

$$\frac{1}{4} \{p_0 + p_1, p_0 + p_1, p_0 - p_1, p_1 - p_0\}. \tag{9.9}$$

Geometrically, this family shown in Fig. 6 may be thought of as a phantom image of the edges of the tetrahedron.

The second and third extraordinary forms describe the family (pure) \otimes (mixed) and (mixed) \otimes (pure), both of which are represented by the apex of the cone.

¹³ Using Eq. (9.8) one may demonstrate the correctness of the corollary also for extraordinary states.

10. Measure and distillation of entanglement

The four-dimensional description of the LSL equivalence classes of two qubits is faithful to the measure of entanglement. (This is not true for the three-dimensional description in [28].) This allows us to give a geometric interpretation of the notion of concurrence and optimize distillation.

10.1. Concurrence as the best evidence

A natural way to quantify entanglement is to measure the expected values of entanglement witnesses [29]. Given an entangled state ρ , the entanglement evidence given by the expectation of the optimal witness is

$$C(\rho) = -\inf_W 2\text{Tr}(W\rho) = -8 \inf_w w^\mu r_\mu = 2(-r_0 + |r_1| + |r_2| + |r_3|). \tag{10.1}$$

The set W in this definition is the set of witnesses with a *normalized representer*. For a separable state the r.h.s. of Eq. (10.1) is clearly negative and one simply defines $C(\rho) = 0$. It is clear from its definition that $C(\rho)$ is a positive quantity if and only if the state ρ is entangled. It can be interpreted geometrically as the distance from the octahedral cone of separable state and it vanishes, of course, on its faces. It is clearly an LSL invariant. This is illustrated in Fig. 7.

Choosing the representative of the state r in the fundamental domain, Eq. (9.7), we have

$$C(\rho) = 2(-r_0 + r_1 + r_2 + |r_3|)_+ = 2(-r_0 + r_1 + r_2 - r_3)_+ = (\rho_0 - \rho_1 - \rho_2 - \rho_3)_+, \tag{10.2}$$

where we use the notation

$$(x)_+ = \begin{cases} x, & x > 0; \\ 0, & \text{otherwise.} \end{cases} \tag{10.3}$$

In the second equality of (10.2) we have used the fact that for any state $(r_0 - r_1 - r_2 - r_3) = \rho_3 > 0$. The r.h.s. is the standard definition of concurrence [51].

10.2. Entanglement distillation

Entanglement is easy to destroy (by mixing) and impossible to increase by local operations. However, one can sometimes distill entanglement by local operations at the price of losing some of the qubits [48]. We have seen in Section 5.2 that one can distill Bell states from a pure mixed state with finite success probability. Here we shall establish a bound on the maximal entanglement one can distill from a *single* mixed state with finite probability. This should be distinguished from the more common distillation protocols, say [6], which rely on operations on multiple identical copies of the state.

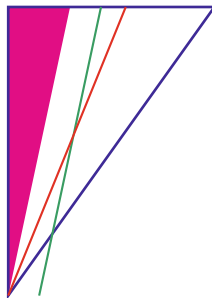


Fig. 7. The pink triangle is the cone of separable states. The green line is a line of constant concurrence. Concurrence increases towards the right. The enclosing blue triangle illustrates the cone of states. States represented by the intersection of the red and green lines can be filtered along the red line. All states can be filtered to have zero entanglement, but in general not to maximal entanglement. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this paper.)

Single copy distillation actually appears as a preliminary step in more general multi-copy protocols [21].

Geometrically, the results are summarized in Fig. 7. More precisely

Theorem 10.1. *Let $C(\rho) > 0$ be the concurrence of the state ρ and let M be the LSL transformation that takes it into its canonical diagonal form. The optimally distilled state is*

$$\rho_f = \frac{M\rho M^\dagger}{\text{Tr}(M\rho M^\dagger)}. \tag{10.4}$$

Its concurrence is

$$C(\rho_f) = \frac{C(\rho)}{4r_0(\rho)} = \frac{(\rho_0 - \rho_1 - \rho_2 - \rho_3)_+}{\rho_0 + \rho_1 + \rho_2 + \rho_3} \geq C(\rho), \tag{10.5}$$

and the distillation succeeds with probability $p(\rho)$

$$p(\rho)C(\rho_f) = \frac{C(\rho)}{\|M\|^2} \leq C(\rho). \tag{10.6}$$

Proof. By the LSL invariance of the concurrence $C(\rho^M) = C(\rho)$. It is then clear from Eq. (10.4) that the concurrence of the renormalized filtered state ρ_f is maximal exactly when $\text{Tr}(M\rho M^\dagger)$ takes its minimal value $4r_0(\rho)$, which occurs precisely when ρ_f is self-dual, by Theorem 7.2. This establishes the optimal concurrence. The probability that distillation succeeds is computed as in Eq. (5.5). \square

Since $0 < 4r_0 \leq 1$ the entanglement always increases, except for the states with $4r_0 = 1$. These are the states represented by the cap of the cone, i.e. entanglement cannot be distilled when the subsystems are fully mixed. On the other hand, pure states have $\rho_j = 0$ and thus can be filtered to be maximally entangled.

11. The Peres–Horodecki separability test

The geometric description of the world of two qubits allows for a simple proof, essentially by inspection, of the “if” part of Theorem 3.2. A similar elementary geometric proof is given in [28].

By Eq. (3.6), partial transposition acts on operators in canonical form as the reflection about the $\sigma_3^{\otimes 2}$ axis. States satisfying the Peres test are then those belonging to the intersection of the tetrahedron with its reflection which is precisely the octahedron of separable states. This shows that a state that satisfies the Peres test must be separable.

The original proof of this fact [23] is algebraic in character, more powerful, and not completely elementary. An elegant version of it also follows from the Choi–Jamiolwosky isomorphism [12] and an alternate simple proof is given in [48].

Acknowledgments

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Appendix A. The existence of a minimizer

To extend Theorem 7.1 to the boundary one needs a stronger version of Lemma 7.4:

Lemma A.1.

- Suppose ρ and W both lie in the interior of the cone of potential witnesses, i.e. satisfying a strict inequality in (8.1). Then, the function $\text{Tr}(\rho W^M)$ diverges to $+\infty$ as either $M_A \in \text{SL}(2, \mathbb{C})$ or $M_B \in \text{SL}(2, \mathbb{C})$ go to infinity. In particular, it has a finite minimizer.
- For any ρ and W in the cone of potential witnesses (boundary included), the function $\text{Tr}(\rho W^M)$ has a finite lower bound.
- Suppose ρ satisfies a strict inequality (8.1) while W satisfies only a weak one. In this case the infimum may be reached for infinite M . However, the corresponding W^M is still guaranteed to have a finite limit.

Proof. Writing the potential witnesses A, B in terms of their associated Lorentz tensors one has $\frac{1}{4}\text{Tr}(AB^{M_1 \otimes M_2}) = (A)^{\mu\nu} (A_1 B A_2)_{\mu\nu}$. We would like to consider the behavior of this expression when the Lorentz transformations $A_1, A_2 \in \text{SO}_+(1, 3)$ involve large boosts.

Any Lorentz transformation A may be written as a combination of a boost of some rapidity t and a rotation. It is then always possible to express A as

$$A(t) = e^t A_+ + e^{-t} A_- + A_0.$$

Moreover, one may write $A_+ = v_+ \otimes u_+, A_- = v_- \otimes u_-, A_0 = v_{0,[1]} \otimes u_{0,[1]} + v_{0,[2]} \otimes u_{0,[2]}$ where $\{u_+, u_-, u_{0,[1]}, u_{0,[2]}\}, \{v_+, v_-, v_{0,[1]}, v_{0,[2]}\}$ are two “light cone” bases of space–time. In the following it will be convenient not to bother with the distinction between the two spatial vectors $u_{0,[1]}, u_{0,[2]}$ (or $v_{0,[1]}, v_{0,[2]}$) and we will usually refer to both of them as u_0 (or v_0) with the extra index implicit.

Expressing the two Lorentz transformations as above one may write

$$(A)^{\mu\nu} (A_1 B A_2)_{\mu\nu} = \sum_{\alpha, \beta} e^{\alpha t_1} e^{\beta t_2} \left(u_\beta^{(2)} \cdot A v_\alpha^{(1)} \right) \left(u_\alpha^{(1)} \cdot B v_\beta^{(2)} \right),$$

where α, β run over the three values $+, -, 0$. Using obvious notations this may be written more shortly as $\sum_{\alpha, \beta} e^{\alpha t_1} e^{\beta t_2} A_{\beta\alpha} B_{\alpha\beta}$.

Consider the case where both $t_1, t_2 \rightarrow \infty$. It is clear that in this limit our function is dominated by the $(\alpha, \beta) = (+, +)$ term: $f \simeq e^{t_1+t_2} A_{++} B_{++}$. Relation (8.1) tells us that $A_{++}, B_{++} \geq 0$. In particular if A, B are strictly in the interior of the cone then they satisfy strict inequality and hence $f \rightarrow +\infty$ proving Part 1 of the lemma.

The second part of the lemma concerns the case where the leading asymptotic term $A_{++} B_{++}$ vanishes. Suppose this is due to $B_{++} = 0$, this means $B v_+^{(2)} \perp u_+^{(1)}$. But we know that $B v_+^{(2)}$ must be in the forward lightcone. This is consistent with $B v_+^{(2)} \perp u_+^{(1)}$ only if $B v_+^{(2)} \propto u_+^{(1)}$, which in turn implies $u_0^{(1)} \cdot B v_+^{(2)} = 0$, i.e. $B_{0+} = 0$. Similarly, one also has $B_{+0} = 0$. We conclude that contributions of the three terms $(\alpha, \beta) = (+, +), (+, 0), (0, +)$ vanish. Since the $(\alpha, \beta) = (+, -), (-, +)$ terms are non-negative while $(\alpha, \beta) = (0, 0), (0, -), (-, 0), (-, -)$ are bounded, one concludes that f has a lower bound proving Part 2 of the lemma.

To check how $A_1 B A_2$ corresponding to B^M behave as $t_1, t_2 \rightarrow \infty$, it is enough to consider its components with respect to the $(t$ -independent!) $\{u\}, \{v\}$ bases, which are just $e^{\alpha t_1} e^{\beta t_2} B_{\alpha\beta}$. We already saw that for the infimum to occur at infinite t one must have $B_{++} = B_{+0} = B_{0+} = 0$. Thus the only terms with the potential to diverge are B_{+-}, B_{-+} . These, however, are strictly non-negative terms and so their divergence would imply $\text{Tr}(AB^M) \rightarrow +\infty$ (assuming $A_{+-}, A_{-+} \neq 0$ for a strict witness A). This phenomenon clearly cannot occur at an infimum of $\text{Tr}(AB^M)$ and thus we conclude that all components of B^M must have a finite limit proving Part 3 of the lemma.

For completeness one should also remark on the case where only one of the t_i 's diverges, say $t_2 \rightarrow \infty$. This may be dealt with similarly to the above by considering the function $A \mapsto \text{Tr}(CA)$ with $C \equiv A A_1 B$ constant. \square

Appendix B. Proof of classification Theorem 8.2

Since the matrix of Lorentz components W maps the forward light-cone into itself, so do W^* and W^*W . The projective space associated with the forward lightcone (i.e. causal four-vectors

modulo normalization) is geometrically a closed three-dimensional ball. Since the closed unit ball is a fixed point domain, [44], the map W^*W must have a fixed point. Let u_0 be the associated direction, and v_0 the corresponding direction for WW^* , i.e.

$$W^*W u_0 = \lambda u_0 \quad WW^* v_0 = \lambda' v_0. \tag{B.1}$$

In fact Wu_0 can be taken as a multiple of v_0 . It then follows $\lambda' = \lambda$ and Wv_0 is a multiple of u_0

$$W u_0 = \sqrt{\lambda} v_0 \quad W^* v_0 = \sqrt{\lambda} u_0. \tag{B.2}$$

There are now four cases. The ordinary case is when u_0 and v_0 are time-like. The three extraordinary cases correspond to the situations when either u_0 or v_0 , or both are light-like.

B.1. The ordinary case

The ordinary case distinguishes two Lorentz frames, one whose time axis coincides with u_0 and another whose time axis coincides with v_0 . Since both vectors are time-like they can be normalized $u_0 \cdot u_0 = v_0 \cdot v_0 = 1$. Let u_j and v_j span the space-like directions corresponding to u_0 and v_0 , respectively. Since

$$v_j \cdot W u_0 = \sqrt{\lambda} v_j \cdot v_0 = 0, \quad v_0 \cdot W u_j = \sqrt{\lambda} u_0 \cdot u_j = 0, \tag{B.3}$$

the pair of Lorentz frames bring W to a form where $W_{0j} = W_{j0} = 0$. The remaining 3×3 spatial block can be diagonalized as in Proposition 6.1, by a pair of spatial rotations, leading to the form (8.10). The condition $w_0 \geq |w_j|$ follows from the requirement that W maps the forward light-cone into itself.

B.2. The second and third extraordinary case

Consider the case where one of causal eigenvectors u_0, v_0 is null.

Suppose $u_0^2 = 1$ but $v_0^2 = 0$. The assumption that WW^* does not have time-like eigenvectors then implies that Wu_0 must be null (or zero). This in turn implies $0 = (Wu_0)^2 = u_0 \cdot W^*Wu_0 = \lambda u_0^2 = \lambda$. Similarly $u_0^2 = 0, v_0^2 = 1$ also implies $\lambda = 0$.

Assume now that $\lambda = 0$ for whatever reason. $W^*Wu_0 = 0$ then implies either $Wu_0 = 0$ or $Wu_0 \propto v_0, W^*v_0 = 0$. Let us concentrate on one of these possibilities, say $W^*v_0 = 0$. It then follows $u \cdot W^*v_0 = 0 \forall u$, i.e. $v_0 \cdot Wu = 0 \forall u$. This relation should hold in particular for any causal vector u , in which case we know that Wu is also causal. However, it is well known that two nonzero vectors both inside the light cone can be orthogonal only if they are a pair of parallel null vectors. We conclude thus that $Wu \propto v_0$. This must hold for any causal u and hence by linearity for all u 's. It follows W is a rank one matrix of the form $v_0 \otimes u$ for some u which is easily identified with u_0 . This means that W is of the form (8.15). The case $Wu_0 = 0$ similarly leads to Eq. (8.14).

B.3. The first extraordinary case

The case of $u_0^2 = v_0^2 = 0$ (and $\lambda \neq 0$) is the hardest one to analyze.

Consider first the case of a self-dual witness A , ¹⁴(e.g. $A = W^*W$) having null eigenvector u_0 . One then has a Jordan block spanned by $\{u_0, u_1, \dots, u_k\}$ such that $Au_i = \lambda u_i + u_{i-1}$ (here $u_{-1} \equiv 0$). It should be noted that there is always some freedom in the choice of the u_i 's. Specifically we may add to u_i any multiple of $u_j, j < i$. Smart choices may help simplifications. We shall make use of the identity $u_i \cdot u_j = u_{i+1} \cdot u_{j-1}$ which follows from the relation $u_i \cdot Au_j = u_j \cdot Au_i$.

- If $k = 1$ then we must have $u_1 \cdot u_0 \neq 0$, for otherwise it cannot span anything outside u_0 . (Other eigenspaces must of course be orthogonal to u_0 .) Taking advantage of our freedom to add to u_1 any multiple of u_0 we may then assume $u_1^2 = 0$. Identifying u_0, u_1 with standard light like vectors $(1, \pm 1, 0, 0)$ we then find A takes the form (8.12) with $w_0 = \lambda, \kappa = \frac{1}{2}$, which is equivalent to “type II” of [17].

¹⁴ This is the case treated in general relativity. Of the four types listed in [17] only the first two satisfy the dominant energy condition.

- If $k = 2$ then $u_1 \cdot u_0 = u_2 \cdot u_{-1} = 0$ imply that u_1 is space-like: $u_1^2 < 0$. We then also have $u_2 \cdot u_0 = u_1^2 \neq 0$ from which it follows that by adding to u_1, u_2 appropriate multiples of u_0 we may assume them to satisfy $u_2^2 = u_2 \cdot u_1 = 0$. It then follows that $Au_2 = \lambda u_2 + u_1$ maps a light-like vector to a spacelike one. This case is therefore not of our interest.
- The $k = 3$ case may be disqualified on the same basis as $k = 2$. However, stronger arguments exist. Note that $u_1^2 = u_3 \cdot u_{-1} = 0$ contradicts $u_1 \cdot u_0 = u_2 \cdot u_{-1} = 0$ (unless $u_1 \propto u_0$). Thus this case cannot arise even if one does not demand A to be a potential witness.

We conclude that only the case $k = 1$ is relevant. Given a non-self-dual W one may then define u_0, u_1 and v_0, v_1 as above corresponding to the self-dual operators $A = W^*W$ and WW^* . Unless $\lambda = 0$ one may pair u_0, v_0 as in Eq. (B.2). Calculation then shows that $Wu_1 - \sqrt{\lambda}v_1$ is an eigenvector of WW^* and hence proportional to v_0 . One may then write:

$$Wu_0 = \sqrt{\lambda}v_0, \quad Wu_1 = \sqrt{\lambda}v_1 + \kappa v_0.$$

Knowing how W acts on u_0 and u_1 essentially solves the classification problem and allows presenting it as in Eq. (8.12).

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