Quantumness and entanglement witnesses

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Abstract

We analyze the recently introduced notion of quantumness witnesses and
compare it to that of entanglement witnesses. We show that any entanglement
witness is also a quantumness witness. We then consider some physically
relevant examples and explicitly construct some witnesses.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The quantal features of a physical system pertain both to its states and observables. States evolve
according to the Schrödinger equation and admit a probabilistic interpretation. Observables
make up an algebra of operators that, in general, do not commute and cannot be simultaneously
measured. Defining quantumness and classicality is an interesting and subtle problem, which
can be tackled from different perspectives, both in physics and mathematics.

Composed quantum systems, made up of two or more subsystems, can be entangled.
Entanglement is a very peculiar quantum characteristic and has become an important resource
in quantum information and quantum applications. Both concepts of entanglement and
quantumness are often investigated by framing them in terms of inequalities: entanglement
and separability are discriminated through the Bell inequality [1], while quantumness and
classicality are discriminated through the Leggett–Garg (LG) inequality [2, 3].

A recent attempt in the study of quantumness and classicality has been made by
Alicki and collaborators [4, 5], who introduced the idea of a 'quantumness witness' (QW),

motivating interesting experiments [6, 7]. Both the theoretical proposal and the experiments mainly focused on single qubits, in the attempt to test their quantum features and rule out (semi)classical descriptions.

In this paper, we shall adopt this approach by focusing on composed systems. We shall propose a combined framework by casting these notions in terms of mathematical definitions and the idea of witnesses. In particular, we shall show that any entanglement witness (EW) is also a QW. To this end, we shall make use of a fully algebraic approach [8, 9].

We shall start by introducing notation and definitions in section 2. The definitions we shall propose are somewhat more general than those of [4, 5]. We show in section 3 that any EW is a QW. Some explicit examples will be worked out in section 4, where we look in particular at the Bell inequality. In section 5, we study the LG inequality and observe that it can also be discussed in the terms of a QW. We conclude with a few remarks in section 6.

2. Classicality, quantumness and entanglement

We introduce notation and define quantumness and entanglement witnesses. We shall only consider finite-dimensional systems.

2.1. Quantumness witnesses

We have the following characterization of commutative (i.e. classical) algebras.

Theorem 1 ([4, 5]). *Given a C*-algebra $\mathcal{A}$, the following two statements are equivalent:*

 (i) $\mathcal{A}$ is commutative. To wit, for any pair $X, Y \in \mathcal{A}$,

$$[X, Y] := XY - YX = 0.$$

(ii) For any pair $X, Y \in \mathcal{A}$ with $X \geqslant 0$ and $Y \geqslant 0$,

$$\{X, Y\} := XY + YX \geqslant 0.$$

As a consequence, for a quantum system one can always find pairs of observables $X \geqslant 0$, $Y \geqslant 0$ such that the observable

$$Q_{\text{AVR}} = \{X, Y\} \tag{1}$$

is *not* positive semidefinite. Thus, $Q_{\text{AVR}} \in \mathcal{A}$ is a 'witness' of the quantumness (i.e. noncommutativity) of the algebra $\mathcal{A}$ [4, 5].

We define classical states, a concept that will be useful in the following.

Definition 1. *We say that a state $\rho \in \mathcal{S}(\mathcal{A})$ is classical if*

$$\rho([X, Y]) = 0, \quad \text{for any pair } X, Y \in \mathcal{A}. \tag{2}$$

A state that is not classical is quantum.

Remark. We recall that the set $\mathcal{S}$ of states of a given algebra $\mathcal{A}$ is the subset of the continuous linear complex functionals $\rho \in \mathcal{A}^*$ (the dual space of $\mathcal{A}$) that are positive and normalized, i.e. $\rho(A^*A) \geqslant 0$ for any $A \in \mathcal{A}$ (A^* being the adjoint), and $\rho(\mathbb{I}) = 1$. See [8, 9].

Remark. Let us also recall that (normal) states $\rho \in \mathcal{S}$ can be *uniquely* realized as traces over density matrices $\tilde{\rho}$ *belonging* to the algebra $\mathcal{A}$:

$$\rho(A) = \text{tr}(\tilde{\rho}A), \qquad \tilde{\rho} \in \mathcal{A}, \quad \tilde{\rho} \geqslant 0, \quad \text{tr}\,\tilde{\rho} = 1. \tag{3}$$

We warn the reader that in the following we will freely use this identification and commit the sin of not distinguishing between states and density matrices.

Note that we can have classical states even when the algebra is noncommutative (namely even when there exist A and B such that $[A, B] \neq 0$). In words, classical states do not 'perceive' nonvanishing commutators. Moreover, the definition (2) of classical state is weaker than the notion of classicality that emerges from (i)–(ii) of theorem 1. Indeed, $\mathcal{A}$ is commutative iff *every* state $\rho \in \mathcal{S}$ is classical.

Remark. Let us note that, in general, mixtures are not classical states. For example, a qubit state $\rho = p|0\rangle\langle0| + q|1\rangle\langle1|$ is not classical, since it possesses coherence, e.g. $\langle-|\rho|+\rangle = c_0 c_1 (p-q)$ for $|+\rangle = c_0|0\rangle + c_1|1\rangle$ and $|-\rangle = c_1^*|0\rangle - c_0^*|1\rangle$, which is nonvanishing provided $p \neq q$ and $c_0, c_1 \neq 0$. On the other hand, the completely mixed state $\rho = \mathbb{I}/2$ is classical, in that it does not possess any coherence, $\langle-|\rho|+\rangle = 0$ for any c_0 and c_1.

Let us now define QWs.

Definition 2. *We say that an observable $Q \in \mathcal{A}$ is a quantumness witness (QW) if*

(i) *for any classical state $\rho \in \mathcal{S}$ one gets $\rho(Q) \geqslant 0$,*
(ii) *there exists a (quantum) state $\sigma \in \mathcal{S}$ such that $\sigma(Q) < 0$.*

The fact that the particular observables Q_{AVR} in (1) are QWs follows from the following lemma.

Lemma 1. *For any classical state $\rho \in \mathcal{S}$ and for any pair $X, Y \in \mathcal{A}$ with $X \geqslant 0$, $Y \geqslant 0$ it happens that*

$$\rho(\{X, Y\}) \geqslant 0. \tag{4}$$

Remark. In words, classical states do not even perceive the possible negativity of the anticommutators $\{X, Y\}$: their behavior is fair with respect to (i)–(ii) of theorem 1.

Proof. Since ρ is classical we get

$$\rho(\{X, Y\}) = \rho(2XY - [X, Y]) = 2\rho(XY). \tag{5}$$

Recall that an observable X is non-negative iff $X = A^*A$ for some $A \in \mathcal{A}$. Therefore,

$$\rho(XY) = \rho(A^*AB^*B) \tag{6}$$

for some $A, B \in \mathcal{A}$. Using again the definition of classicality (2) we conclude

$$\rho(XY) = \rho(BA^*AB^*) = \rho(C^*C) \geqslant 0, \tag{7}$$

with $C = AB^* \in \mathcal{A}$. □

2.2. Entanglement witnesses

Let our system be made up of two *subsystems*, that will conventionally be sent to Alice and Bob, whose observations are independent. The notion of independence is reflected in the fact that the total algebra of observables is assumed to factorize in two subalgebras:

$$\mathcal{C} = \mathcal{A} \otimes \mathcal{B}. \tag{8}$$

Namely, the two subalgebras commute with each other, but each subalgebra can be noncommutative.

Definition 3. *A state $\rho \in \mathcal{S}(\mathcal{C})$ is said to be separable (with respect to the given bipartition $\mathcal{A} \otimes \mathcal{B}$) if it can be written as a convex combination of product states, namely*

$$\rho = \sum_k p_k \rho_k \otimes \sigma_k, \qquad p_k > 0, \qquad \sum_k p_k = 1, \qquad (9)$$

where $\rho_k \in \mathcal{S}(\mathcal{A})$ and $\sigma_k \in \mathcal{S}(\mathcal{B})$ are states of $\mathcal{A}$ and $\mathcal{B}$, respectively. A state that is not separable is said to be entangled (with respect to the given bipartition).

Remark. The definition of separability depends on the algebra $\mathcal{C}$ of the composed system, that in general can be reducible, i.e. the matrices $C \in \mathcal{C}$ are block diagonal, $C = \bigoplus_k C_k$. If states are identified with density matrices belonging to the algebra as in (3), then they inherit the block-diagonal form of the latter.

Definition 4 ([10, 11])**.** *We say that an observable $E \in \mathcal{C}$ is an entanglement witness (EW) if*

 (i) for any separable state $\rho \in \mathcal{S}(\mathcal{C})$ one gets $\rho(E) \geqslant 0$,
 (ii) there exists a (entangled) state $\sigma \in \mathcal{S}(\mathcal{C})$ such that $\sigma(E) < 0$.

3. All EWs are QWs

We now show that every EW is also a QW. We first consider a preliminary lemma.

Lemma 2. *Any classical state is separable.*

Proof. Note first that if the algebra $\mathcal{C} = \mathcal{A} \otimes \mathcal{B}$ is the full algebra of operators

$$\mathcal{C} = B(\mathbb{C}^n) \otimes B(\mathbb{C}^m), \qquad (10)$$

then the only classical state is the totally mixed state,

$$\rho = \mathbb{I}_{nm}/nm = \mathbb{I}_n/n \otimes \mathbb{I}_m/m, \qquad (11)$$

which is obviously separable. In general, however, the (sub)algebras $\mathcal{A}$ and $\mathcal{B}$ are reducible (i.e. they are proper subalgebras of the full matrix algebra) and one has

$$\mathcal{C} = \left(\bigoplus_k B(\mathbb{C}^{n_k})\right) \otimes \left(\bigoplus_l B(\mathbb{C}^{m_l})\right) = \bigoplus_{k,l} B(\mathbb{C}^{n_k}) \otimes B(\mathbb{C}^{m_l}) =: \bigoplus_{k,l} \mathcal{C}_{kl}, \qquad (12)$$

where each $\mathcal{C}_{kl}$ is an irreducible algebra of dimension $n_k m_l$. All observables are block diagonal and the classical states have the form

$$\rho = \bigoplus_{k,l} p_{kl} \mathbb{I}_{n_k}/n_k \otimes \mathbb{I}_{m_l}/m_l, \qquad (13)$$

with $p_{kl} \geqslant 0$ and $\sum_{kl} p_{kl} = 1$, i.e. they are separable. $\square$

Remark. Note that if the two subalgebras are reducible, states inherit their block-diagonal structure. See remark after equation (9).

Our main theorem is now an easy consequence of the lemma just proved.

Proposition 1. *Any EW is a QW.*

Proof. Consider an EW $E \in \mathcal{C}$. By definition $\rho(E) \geqslant 0$ for any separable $\rho \in \mathcal{S}$. But by the previous lemma all classical states are separable. It follows that $\rho(E) \geqslant 0$ for any classical state ρ. Moreover, by definition, $\sigma(E) < 0$ for some entangled state σ, which by the previous lemma must be a quantum state. Thus, E is a QW. $\square$

Remark. The converse is, of course, not true. If the algebra $\mathcal{A}$ is noncommutative, and $Q \in \mathcal{A}$ is a QW of the quantum state $\sigma \in \mathcal{S}(\mathcal{A})$, then

$$\tilde{Q} = Q \otimes \mathbb{I} \in \mathcal{C} \tag{14}$$

is also a QW (of the total algebra), but it is *not* an EW. Indeed, it is negative on separable states of the form $\sigma \otimes \omega$ (for any $\omega \in \mathcal{S}(\mathcal{B})$), namely

$$(\sigma \otimes \omega)(\tilde{Q}) < 0. \tag{15}$$

4. Explicit construction of EWs as anticommutators for qudits

In the previous section, we have shown that an EW is always a QW. In view of that, among all QWs, those of the simple form (1), that we shall call *anticommutator QWs*, are quite interesting for possible applications, for example, for efficiently generating EWs out of anticommutators. Therefore, here we shall investigate whether an EW E can be written in the *particular* form (1), namely whether there exists a pair of positive operators X and Y such that $E = \{X, Y\}$. Before looking at a rather general case, we consider some instructive examples.

4.1. Swap operator and Bell inequality

An example of EW for a $d \times d$ system is the swap operator [11]

$$S = \sum_{i,j=0}^{d-1} |i\rangle\langle j| \otimes |j\rangle\langle i|. \tag{16}$$

Here, the algebra is the full algebra of matrices $B(\mathbb{C}^d) \otimes B(\mathbb{C}^d)$, and $\{|j\rangle\}_j$ is a chosen orthonormal basis of $\mathbb{C}^d$ (computational basis). S is non-negative, $\rho(S) \geqslant 0$, for all separable states ρ, but it possesses an eigenvalue equal to -1.

Another interesting example of EW is the Bell-CHSH observable

$$E_{\text{Bell}} = 2 \pm (A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2), \tag{17}$$

where $A_{1,2} \in \mathcal{A}$ and $B_{1,2} \in \mathcal{B}$ are dichotomic observables (with eigenvalues ± 1) of Alice and Bob, respectively, and $A_{1,2}^2 = \mathbb{I}$, $B_{1,2}^2 = \mathbb{I}$. If $\rho(E_{\text{Bell}}) < 0$, E_{Bell} witnesses the violation of the Bell-CHSH inequality in the entangled state ρ.

For instance, if we take

$$A_1 = \sigma_x, \qquad B_1 = \tfrac{1}{\sqrt{2}}(\sigma_x + \sigma_y),$$
$$A_2 = \sigma_y, \qquad B_2 = \tfrac{1}{\sqrt{2}}(\sigma_x - \sigma_y), \tag{18}$$

where $\sigma_{x,y,z}$ are Pauli operators

$$\sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|, \quad \sigma_y = -\mathrm{i}|0\rangle\langle 1| + \mathrm{i}|1\rangle\langle 0|, \quad \sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|, \tag{19}$$

then

$$E_{\text{Bell}} = 2 \pm \sqrt{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y). \tag{20}$$

Observe now that the swap operator (16) and the Bell-CHSH observable (20) are related by

$$S = P_{00} + P_{11} \pm \tfrac{1}{2\sqrt{2}}(E_{\text{Bell}} - 2), \tag{21}$$

where

$$P_{ij} = |i\rangle\langle i| \otimes |j\rangle\langle j| \qquad (i, j = 0, 1) \tag{22}$$

are projections.

Due to the negative shift -2 in (21), S is more efficient at witnessing entanglement than E_{Bell}: S can actually detect entangled states that do not violate the Bell inequality. For instance, let $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$, then the entanglement of the vector state

$$|\chi\rangle = a|+\rangle \otimes |-\rangle + b|-\rangle \otimes |+\rangle \tag{23}$$

is witnessed by S if $\text{Re}(a^*b) < 0$, while E_{Bell} in equation (20) (with the $+$ sign) is negative only for $\text{Re}(a^*b) < -(\sqrt{2}-1)/2$.

4.2. Reviewing previous results

We now briefly review some results obtained in [5]. Let

$$
\begin{aligned}
X &= 2 \pm (A_1 \otimes B_1 + A_1 \otimes B_2) \geqslant 0, \\
Y &= 2 \pm (A_2 \otimes B_1 - A_2 \otimes B_2) \geqslant 0,
\end{aligned}
\tag{24}
$$

with dichotomic observables $A_{1,2} \in \mathcal{A}$, $B_{1,2} \in \mathcal{B}$. One easily gets

$$
\begin{aligned}
XY &= 2E_{\text{Bell}} + (A_1A_2 \otimes B_2B_1 - A_1A_2 \otimes B_1B_2), \\
YX &= 2E_{\text{Bell}} + (A_2A_1 \otimes B_1B_2 - A_2A_1 \otimes B_2B_1).
\end{aligned}
\tag{25}
$$

If the algebra $\mathcal{A}$ of Alice *or* the algebra $\mathcal{B}$ of Bob is *commutative*, the sum of the terms in brackets in (25) cancel and

$$Q_{\text{AVR}} = \{X, Y\} = 4E_{\text{Bell}}. \tag{26}$$

As explained in section 2.1, since $[X, Y] = 0$ and $X, Y \geqslant 0$, their symmetrized product must also be non-negative: $Q_{\text{AVR}}/4 = E_{\text{Bell}} \geqslant 0$. This is the Bell-CHSH inequality.

On the other hand, if the subalgebras $\mathcal{A}$ and $\mathcal{B}$ of Alice and Bob are *both* noncommutative, one obtains

$$Q_{\text{AVR}} = \{X, Y\} = 4E_{\text{Bell}} - [A_1, A_2] \otimes [B_1, B_2], \tag{27}$$

which coincides with the result obtained in [5] modulo a factor 2. The above expression, with the choice of operators as in (18), turns out to be *positive semidefinite* for any Bell state. Therefore, Q_{AVR} is not witnessing entanglement. Q_{AVR} can be shown to be negative for suitable factorized states, so it tests the quantumness of the individual subsystems.

4.3. The Bell-CHSH inequality is also an anticommutator QW

Let

$$
\begin{aligned}
X &= 2 \pm (A_1 \otimes B_1 - A_2 \otimes B_2) \geqslant 0, \\
Y &= 2 \pm (A_1 \otimes B_2 + A_2 \otimes B_1) \geqslant 0,
\end{aligned}
\tag{28}
$$

which are symmetric under the exchange $A \leftrightarrow B$, in contrast to those in (24). Then,

$$
\begin{aligned}
XY &= 2E_{\text{Bell}} + [A_1, A_2] \otimes \mathbb{I} + \mathbb{I} \otimes [B_1, B_2], \\
YX &= 2E_{\text{Bell}} - [A_1, A_2] \otimes \mathbb{I} - \mathbb{I} \otimes [B_1, B_2],
\end{aligned}
\tag{29}
$$

so that

$$Q_{\text{AVR}} = \{X, Y\} = 4E_{\text{Bell}}. \tag{30}$$

This shows that the EW E_{Bell} is also an anticommutator QW: if the Bell-CHSH inequality is violated by an entangled state ρ, then $\rho(Q_{\text{AVR}}) < 0$.

An interesting remark is the following one: assume you have two particles, on which Alice and Bob measure dichotomic observables. They put together their results and find that

a state ρ exists such that $\rho(E_{\text{Bell}}) < 0$. Then they can conclude that their local observables do not commute.[8] In this sense, one can say that the Bell inequality is testing quantumness and not simply entanglement: by looking only at the correlations of the two subsystems, one can check whether the two local (sub)algebras are noncommutative.

4.4. A more general case

Let us consider a more general case, i.e. the swap operator S defined in (16) for a pair of qudits. For a pair of qubits, it reads in the basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ (here $|jk\rangle := |j\rangle \otimes |k\rangle$)

$$
S = \begin{pmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{pmatrix},
\tag{31}
$$

and for a pair of qutrits (in the basis $\{|00\rangle, |01\rangle, |10\rangle, |02\rangle, |20\rangle, |11\rangle, |12\rangle, |21\rangle, |22\rangle\}$),

$$
S = \begin{pmatrix} 1 & & & & & & & & \\ & 0 & 1 & & & & & & \\ & 1 & 0 & & & & & & \\ & & & 0 & 1 & & & & \\ & & & 1 & 0 & & & & \\ & & & & & 1 & & & \\ & & & & & & 0 & 1 & \\ & & & & & & 1 & 0 & \\ & & & & & & & & 1 \end{pmatrix}.
\tag{32}
$$

In this way, for a generic $d \times d$ system, S is block diagonal and contains 2×2 blocks

$$
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\tag{33}
$$

and these yield negative eigenvalues equal to -1. The explicit construction of EWs of the form (1) for qudits is therefore reduced to understanding whether there exists a pair of positive operators X and Y ($X, Y \geqslant 0$) such that

$$
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \stackrel{?}{=} \{X, Y\}
\tag{34}
$$

sector by sector. It is trivial to construct X and Y for the diagonal elements 1 in equation (31) or (32).

4.4.1. Q_{AVR} for a generic two-state system.
Let us first determine the eigenvalues of a QW of the type (1) for a two-state system. Generic positive operators X and Y of a two-state system can be expressed as

$$
X = \tfrac{1}{2}\alpha(1 + \boldsymbol{u} \cdot \boldsymbol{\sigma}), \qquad Y = \tfrac{1}{2}\beta(1 + \boldsymbol{v} \cdot \boldsymbol{\sigma}),
\tag{35}
$$

with vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, respectively, whose lengths are limited by

$$
0 \leqslant u, v \leqslant 1,
\tag{36}
$$

and with positive constants $\alpha, \beta > 0$ (we exclude $\alpha, \beta = 0$, since we are interested in nontrivial operators). The anticommutator QW is then given by

$$
Q_{\text{AVR}} = \{X, Y\} = \tfrac{1}{2}\alpha\beta[1 + \boldsymbol{u} \cdot \boldsymbol{v} + (\boldsymbol{u} + \boldsymbol{v}) \cdot \boldsymbol{\sigma}]
\tag{37}
$$

---

[8] In this case, *both* algebras $\mathcal{A}$ and $\mathcal{B}$ are noncommutative. Indeed, it is easy to prove that if one of the two algebras were classical then any state ρ of the composed system would necessarily be separable. See e.g. proposition 2.5 in [12].
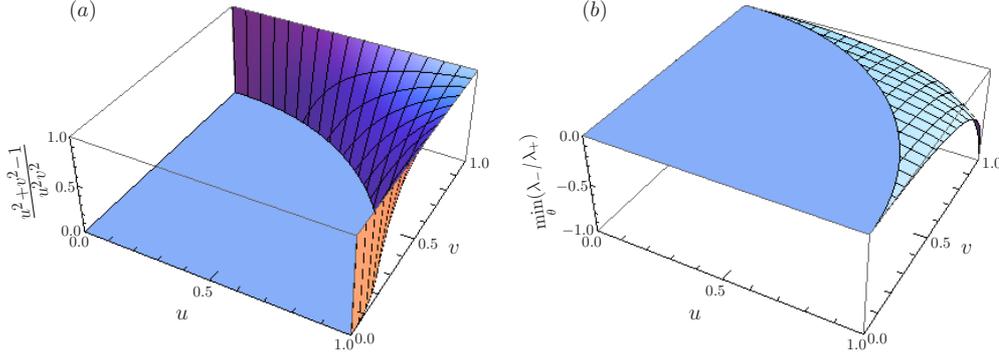
Figure 1. (*a*) $(u^2 + v^2 - 1)/u^2 v^2$ as a function of (u, v), yielding the upper bound on $\cos^2 \theta$ for each (u, v). See (40). If θ violates this bound, $Q_{\text{AVR}} = \{X, Y\}$ in (37) is no longer a QW. In the region where this upper bound is negative, Q_{AVR} can never be a QW. Therefore, only the positive range is shown. (*b*) Smallest attainable ratio $\min_\theta (\lambda_- / \lambda_+)$ of the eigenvalues in (38) as a function of (u, v). λ_- / λ_+ should be strictly negative for Q_{AVR} to be a QW. Therefore, only the negative range is shown. The ratio λ_- / λ_+ can come close to -1 only when $u = v = 1$.

and admits two eigenvalues

$$\lambda_\pm = \tfrac{1}{2}\alpha\beta(1 + \boldsymbol{u} \cdot \boldsymbol{v} \pm |\boldsymbol{u} + \boldsymbol{v}|), \tag{38}$$

the corresponding eigenstates $|\lambda_\pm\rangle$ being the two eigenstates of the operator $(\boldsymbol{u} + \boldsymbol{v}) \cdot \boldsymbol{\sigma}$.

In order for (37) to be a QW, one must have $\lambda_- < 0$. This entails

$$1 + \boldsymbol{u} \cdot \boldsymbol{v} < |\boldsymbol{u} + \boldsymbol{v}|, \tag{39}$$

which yields the condition

$$\cos^2 \theta < \frac{u^2 + v^2 - 1}{u^2 v^2}, \tag{40}$$

where θ is the angle between the two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ and $\boldsymbol{u} \cdot \boldsymbol{v} = uv \cos \theta$. See figure 1(*a*) for the range of $(u^2 + v^2 - 1)/u^2 v^2$. See also figure 1(*b*), where the smallest attainable ratio λ_- / λ_+ is displayed as a function of (u, v). This shows that the $u = v = 1$ case covers the widest range of eigenvalues (λ_+, λ_-).

Let us thus fix $u = v = 1$. In this case, the two eigenvalues $\lambda_\pm$ of Q_{AVR} read

$$\lambda_+ = 2\alpha\beta \cos \frac{\theta}{2} \cos^2 \frac{\theta}{4}, \quad \lambda_- = -2\alpha\beta \cos \frac{\theta}{2} \sin^2 \frac{\theta}{4} \quad (0 < \theta < \pi). \tag{41}$$

Note that $\theta = 0$ and π are excluded, since λ_- vanishes at these points. The sum and ratio of the two eigenvalues read

$$\lambda_+ + \lambda_- = 2\alpha\beta \cos^2 \frac{\theta}{2}, \qquad \frac{\lambda_-}{\lambda_+} = -\tan^2 \frac{\theta}{4}, \tag{42}$$

respectively. In particular, the ratio ranges between

$$-1 < \frac{\lambda_-}{\lambda_+} < 0. \tag{43}$$

4.4.2. S is almost $Q_{\text{AVR}} = \{X, Y\}$. Let us now consider a relevant 2×2 sector of S, and try to construct positive operators X and Y such that $S = \{X, Y\}$ *in the sector*. The eigenvalues of S in each relevant 2×2 sector are 1 and -1, whose ratio is -1. Since the ratio of the eigenvalues $\lambda_\pm$ of the QW (37), for a two-state system, can only range between $-1 < \lambda_- / \lambda_+ < 0$ as

in (43), there is no hope of constructing X and Y. In this sense, the EW S *cannot* be written as an anticommutator QW. However, if we add to S a part proportional to the identity

$$S \to \xi \mathbb{I} + S, \tag{44}$$

the situation changes. In such a case, the eigenvalues are shifted to

$$1 + \xi \quad \text{and} \quad -1 + \xi. \tag{45}$$

Note first that in order for this to remain an EW, ξ should be bounded by $\xi < 1$; otherwise, we lose the negative eigenvalue and $\xi \mathbb{I} + S$ is no longer an EW. In addition, from (43), the ratio of the shifted eigenvalues should be bounded by

$$-1 < -\frac{1-\xi}{1+\xi} < 0, \tag{46}$$

in order for $\xi \mathbb{I} + S$ to be expressed as an anticommutator, $\xi \mathbb{I} + S = \{X_\xi, Y_\xi\}$. This requires $\xi > 0$. Therefore, ξ should be bounded by

$$0 < \xi < 1 \tag{47}$$

in order for $\xi \mathbb{I} + S$ to be an EW and at the same time an anticommutator QW.

Let us construct X_ξ and Y_ξ explicitly, with the lengths of the associated vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ being $u = v = 1$. The angle θ between the two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ is fixed by the condition

$$\frac{\lambda_-}{\lambda_+} = -\frac{1-\xi}{1+\xi} = -\tan^2 \frac{\theta}{4}. \tag{48}$$

See (42). Hence,

$$\xi = \cos \frac{\theta}{2}, \tag{49}$$

and

$$\begin{cases} \boldsymbol{u} = (\sqrt{1-\xi^2} \cos \varphi, \sqrt{1-\xi^2} \sin \varphi, \xi), \\ \boldsymbol{v} = (-\sqrt{1-\xi^2} \cos \varphi, -\sqrt{1-\xi^2} \sin \varphi, \xi), \end{cases} \tag{50}$$

where φ is an arbitrary parameter $0 \leqslant \varphi < 2\pi$, and the z direction is chosen in the direction of $\boldsymbol{u} + \boldsymbol{v}$, i.e.

$$\sigma_z = \frac{\boldsymbol{u} + \boldsymbol{v}}{|\boldsymbol{u} + \boldsymbol{v}|} \cdot \boldsymbol{\sigma} = |\lambda_+\rangle\langle\lambda_+| - |\lambda_-\rangle\langle\lambda_-|,$$

$$\sigma_x = |\lambda_+\rangle\langle\lambda_-| + |\lambda_-\rangle\langle\lambda_+|, \qquad \sigma_y = -i|\lambda_+\rangle\langle\lambda_-| + i|\lambda_-\rangle\langle\lambda_+|. \tag{51}$$

See figure 2. On the other hand, by plugging (49) into the first relation in (42), one has

$$\lambda_+ + \lambda_- = 2\xi = 2\alpha\beta \cos^2 \frac{\theta}{2} = 2\alpha\beta\xi^2, \tag{52}$$

which yields

$$\alpha\beta = \frac{1}{\xi}. \tag{53}$$

Therefore, by (51) we obtain

$$X_\xi, Y_\xi = \frac{1}{2\sqrt{\xi}} \left[(1+\xi)|\lambda_+\rangle\langle\lambda_+| + (1-\xi)|\lambda_-\rangle\langle\lambda_-| \right. \tag{54}$$

$$\left. \pm \sqrt{1-\xi^2} (e^{-i\varphi}|\lambda_+\rangle\langle\lambda_-| + e^{i\varphi}|\lambda_-\rangle\langle\lambda_+|) \right]. \tag{55}$$
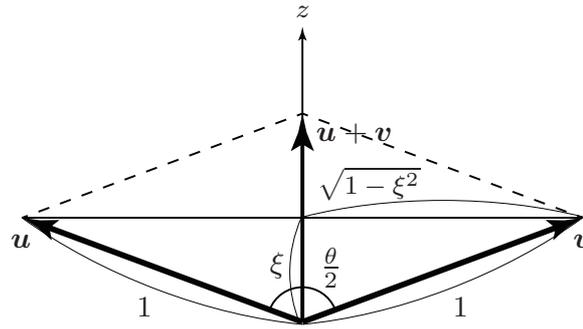
Figure 2. Arrangement of *u* and *v* for $\xi\mathbb{I} + S = \{X_\xi, Y_\xi\}$.

In particular, for a pair of qubits, we have $|\lambda_\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$, so that

$$\xi\mathbb{I} + S = \begin{pmatrix} \xi+1 & 0 & 0 & 0 \\ 0 & \xi & 1 & 0 \\ 0 & 1 & \xi & 0 \\ 0 & 0 & 0 & \xi+1 \end{pmatrix}, \tag{56}$$

and

$$X_\xi, Y_\xi = \begin{pmatrix} \sqrt{\dfrac{1+\xi}{2}} & 0 & 0 & 0 \\ 0 & \dfrac{1\pm\sqrt{1-\xi^2}\cos\varphi}{2\sqrt{\xi}} & \dfrac{\xi\pm\mathrm{i}\sqrt{1-\xi^2}\sin\varphi}{2\sqrt{\xi}} & 0 \\ 0 & \dfrac{\xi\mp\mathrm{i}\sqrt{1-\xi^2}\sin\varphi}{2\sqrt{\xi}} & \dfrac{1\mp\sqrt{1-\xi^2}\cos\varphi}{2\sqrt{\xi}} & 0 \\ 0 & 0 & 0 & \sqrt{\dfrac{1+\xi}{2}} \end{pmatrix}. \tag{57}$$

Therefore, we obtain

$$S = \{X_\xi, Y_\xi\} - \xi\mathbb{I}, \qquad 0 < \xi < 1. \tag{58}$$

Since the positive shift ξ can be arbitrarily small, the EW S is almost (but not quite) an anticommutator QW. X_ξ and Y_ξ can be constructed in the same manner for higher dimensional systems, sector by sector.

5. The Leggett–Garg inequality

We conclude this note by discussing the LG inequality [2, 3] and an interesting connection with the approach taken in this paper. Let $Z(t)$ be a time-dependent dichotomic variable, with spectrum $\{-1, +1\}$. Under the assumption of macrorealism and noninvasive measurability of the system's state, a macroscopic object, with two macroscopically distinct states, is at any given time in a definite one of these states (corresponding to the measurement value $Z = \pm 1$) and it is possible to determine which of these states the system is in without any effect on the state itself, or on the subsequent system dynamics. Under these assumptions, Leggett and Garg [2] proved that

$$1 - Z_0 Z_1 - Z_1 Z_2 + Z_0 Z_2 \geqslant 0, \tag{59}$$

where $Z_j = Z(t_j)$ and we assume $t_0 < t_1 < t_2$. We start by giving an operational meaning to the above quantity. It is constructed in terms of time correlations of the observable Z and it involves 'snapshots' of this observable at different instants of time. Like in a Bell inequality, several measurements are needed in order to ascertain the average value of each product appearing in (59). We take

$$\rho(Z_0 Z_1) = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} Z_0^{(j)} Z_1^{(j)}, \tag{60}$$

where $Z_0^{(j)}$ and $Z_1^{(j)}$ are the experimental outcomes of the observables Z_0 and Z_1, respectively, in the jth ($j = 1, \ldots, N$) experimental run on systems all prepared in the same state ρ [8]. Similar relations hold for the other products in (59).

The first question is as follows. Is it possible to write (59) as the product of two positive numbers? Assume that the observables of the system commute (this embodies the afore-mentioned notion of noninvasive measurability) and define

$$X = 1 - Z_0 Z_1 \geqslant 0,$$
$$Y = 1 - Z_1 Z_2 \geqslant 0. \tag{61}$$

Then

$$XY = 1 - Z_0 Z_1 - Z_1 Z_2 + Z_0 Z_2,$$
$$YX = 1 - Z_0 Z_1 - Z_1 Z_2 + Z_1 Z_2 Z_0 Z_1 = 1 - Z_0 Z_1 - Z_1 Z_2 + Z_0 Z_2 = XY, \tag{62}$$

the second chain of equalities being valid because the algebra of the system is commutative. We therefore obtain

$$C = \{X, Y\} = 2(1 - Z_0 Z_1 - Z_1 Z_2 + Z_0 Z_2) \geqslant 0, \tag{63}$$

which is the LG inequality.

A few words of caution are in order. In evaluating YX in (62) one encounters the quantity $Z_1 Z_2 Z_0 Z_1$, whose operational meaning according to (60) is

$$\rho(Z_1 Z_2 Z_0 Z_1) = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} Z_1^{(j)} Z_2^{(j)} Z_0^{(j)} Z_1^{(j)} = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} Z_2^{(j)} Z_0^{(j)} = \rho(Z_0 Z_2) \tag{64}$$

for any state ρ, where we used $Z_1^{(j)} = \pm 1$. We see that one need not measure Z_1 in order to obtain $Z_0 Z_2$. Observe that this would not be valid in quantum mechanics. A measurement at time t_1 would perturb the system and affect the outcome at time t_2. As a result, the correlation $\rho(Z_0 Z_2)$ would differ from the one estimated without performing the measurement at t_1. It is also manifested from the above discussion that the notion of commutativity of the observables and noninvasive measurability are intertwined in this framework.

If the LG inequality (63) is violated, at least one of the premises of the above reasoning is not valid, and we can say that the (macroscopic) system is quantum. As a byproduct, we have expressed the LG quantity that appears in (63) as an anticommutator QW.

In the noncommutative case the operators X and Y in (61) are not positive, and not even Hermitian. Define

$$X = 1 - Z_0 \circ Z_1 \geqslant 0,$$
$$Y = 1 - Z_1 \circ Z_2 \geqslant 0, \tag{65}$$

where $A \circ B = \{A, B\}/2$ is the symmetrized (Jordan) product. Then

$$XY = 1 - Z_0 \circ Z_1 - Z_1 \circ Z_2 + (Z_0 \circ Z_1)(Z_1 \circ Z_2),$$
$$YX = 1 - Z_0 \circ Z_1 - Z_1 \circ Z_2 + (Z_1 \circ Z_2)(Z_0 \circ Z_1). \tag{66}$$

Thus,

$$C = \{X, Y\} = 2[1 - Z_0 \circ Z_1 - Z_1 \circ Z_2 + (Z_0 \circ Z_1) \circ (Z_1 \circ Z_2)]. \tag{67}$$

This is the quantity to test in a quantum experiment. Clearly, if we assume that the algebra of the system is commutative, then $A \circ B = AB = BA$ and we reobtain (63).

Note that the logical status of this inequality is different from that of the Bell inequality discussed in section 4. In the case discussed in this section, one is not detecting entanglement, but rather the symptoms of nonclassicality in a single (macroscopic) quantum system.

6. Conclusions and perspectives

We have discussed the notions of quantumness and entanglement, showing that every entanglement witness is also a quantumness witness. Although entanglement is clearly a genuine quantum feature, our analysis makes use of strict mathematical definitions of witnesses. This enables one to put (physical) intuition on firm mathematical grounds. In turn, theorems and their derivations disclose alternative viewpoints: we observed in section 4.3 that the Bell inequality, written as a QW, tests the 'global' quantumness of the composed system. This enables one to look at the Bell inequality from a novel perspective.

An interesting aspect that could be investigated in the future is whether the combined notions of quantumness and entanglement witnesses could shed light on the elusive notion of bound entanglement [13, 14], for which the partial transpose (PT) criterion does not apply.

We conclude by noting that the links between nonclassicality and entanglement have also been investigated in quantum optics [15]. At the root of this approach there is the idea that the PT of some positive operators can detect nonclassicality in the light fields, witnessing it through suitable Cauchy– Schwarz inequalities [16]. Also, the notion of 'partial' quantumness/classicality, suitably defined in order to provide a finer graining between the quantum and classical worlds, can be shown to incorporate an ordering relation among different nonclassical correlations and entanglement measures [17]. In this analysis, which makes extensive use of inequalities, the focus is on the quantum-to-classical transition. Although the language used in the above-mentioned investigations is slightly different from that used in this paper, the links between these methods are worth exploring in the future.

Finally, an aspect of interest would be to analyze the relation between the present approach and the definition of classicality based on the positivity of the Glauber–Sudarshan *P*-representation [18, 19]. Such a representation uses the coherent states as a basis, and for this reason has a straightforward semiclassical description [20, 21].

The extension of our definitions to infinite-dimensional systems, such as coherent states, superpositions thereof and in general two-mode light states, as well as a discussion of the semiclassical limit, is left for the future. In this framework, the notions of classicality and quantumness are in opposition, and to obtain the former as a limit of the latter is an interesting challenge.

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