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Bell-CHSH non-locality and entanglement from a unified framework

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Abstract. Non-classical probability is a defining feature of quantum mechanics. This paper develops a formalism that exhibits explicitly, the manner in which rules of classical probability break down in the quantum domain. Thereby, a framework is set up which allows for construction of signatures for non-classicality of states in a systematic manner. Using this, conditions for non-locality and entanglement are shown to emerge from a break down of classical probability rules. Bell-CHSH non-locality is derived for any bipartite systems and entanglement inequalities are obtained for coupled two level systems only.

1 Introduction

Quantum mechanics has altered the very way we comprehend laws of nature. Equally so, it has altered the way we formulate laws of probability. Thus, the concept of non-classicality of states in quantum physics is as much a reflection of the new probability as it is of non-classical physics. Recent developments in quantum information have brought the realization that non-classicality of quantum states can, in fact, act as resources for information processing, some of which could even be impossible otherwise [1,2]. In consequence, many definitions and criteria have been proposed [3–13]. In parallel, there has been a vigorous experimental activity, both for probing the foundations of quantum mechanics [14–17] and for eminently practical applications [1,18–20].

Spectacular though these developments are, our present understanding of non-classicality is not entirely satisfactory. Each definition/criterion is pinned to a specific scenario, and its interrelationship with other criteria is not always clear. A formalism that defines non-classicality directly in the language of quantum probability, and is also inherently quantifiable, would bridge this gap. It would also allow a systematic way of devising tests of non-classical features of a quantum state.

This paper accomplishes that task. It does so by constructing quantum representatives of indicator functions defined for supports for outcomes of classical observables, in the phase space, and the intersections, unions and complements thereof. Indicator functions are, by definition, classical observables. Though all the indicator functions (corresponding to intersections, unions and complements) are of equal importance, only the first operation has received attention [21–31]. We call these representatives pseudo projections.

Pseudo projections hold the key to non classicality. They are shown to yield an infinitely large number of tests of non-classicality of states. In particular, as an important application, we demonstrate the emergence of Bell-CHSH non-locality (in any dimension) and a series of entanglement inequalities (for two qubit systems) from a single unifying formalism. Keeping this practical perspective in mind, we do not wade into the more complicated and unresolved issues concerning the logical foundations of quantum mechanics or of quantum probability.

The paper is organised as follows. Section 2 establishes the framework. In Sections 3–4, methods of constructing pseudo projections representing indicator functions associated with classical events are developed. In Section 5, we define non-classicality conditions on a state with respect to a given set of observables. Section 6, which has results central to this paper, demonstrates the emergence of Bell CHSH non-locality, and a set of inequalities that form a chain of sufficiency conditions for entanglement. The quantitative features of the inequalities are discussed in Section 7. Section 8 concludes the paper with some closing remarks.

2 The framework

As a preliminary, we first discuss the case of outcomes of a single observable.

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2.1 Indicator functions for single outcomes and their quantum representatives

We start with classical observables $A, B, \cdots$ defined over a phase space Φ[1]. Let $S_i^A \subset \Phi$ be the support for the outcome $A = a_i$. Similarly, let $S_j^B \subset \Phi$ be the support for the outcome $B = b_j$. If a system is in a state f, the respective probabilities for the outcomes will be given by the overlap of f with the corresponding indicator functions $I_{S_i^A}$ and $I_{S_j^B}$. The indicator functions are Boolean observables, taking the value 1 within the support and zero outside. For a given observable, the supports S_i are mutually disjoint, and partition Φ: $S_i \bigcap S_j = \emptyset$ (the null space); $\bigcup_i S_i = \Phi$.

Consider the transition to the quantum domain. The phase space maps to a Hilbert space $\mathcal{H}$, and a classical state – to a density operator ρ. An observable A maps to a self adjoint operator denoted, again, by A which admits the spectral decomposition, $A = \sum_i a_i \pi_i^A$; the eigen projections π_i^A partition $\mathcal{H}$ into a disjoint union of subspaces, $\mathcal{H} = \bigcup_i \oplus \mathcal{H}_i^A$. Finally, the probability for the outcome $A = a_i$ is given by the overlap, $p_i^A = Tr(\rho \pi_i^A)$. All other outcomes are disallowed.

Two important mappings that follow are of particular relevance. Let S be the support of a classical outcome a of an observable A, and I_S be its indicator function. From the rule stated above, there exists a subspace $\mathcal{H}_S$, projected by a projection π, governed by $I_S \to \pi; S \to \mathcal{H}_S$. However, if a is not an eigenvalue of A, then $\mathcal{H}_S$ is the trivial null space $\emptyset$ and the projection $\pi = \mathbf{0}$, the null operator.

The situation changes when multiple observables are considered. We now ask for quantum representatives of the indicator functions constructed over intersections, unions and complements of the respective supports. Non classical features are embedded inherently in the properties of these quantum representatives, as we show in this paper. We call them pseudo projections. Pseudo projections become projections only when the algebra of the observables considered is abelian.

3 Pseudo projections that represent indicator functions for joint outcomes

We start with the construction of pseudo projections representing indicator functions that correspond to joint outcomes of observables. We essentially rederive the expressions proposed in [30], but in a language that is more amenable to construction of pseudo-projection representing indicator functions defined over union and complement of supports. Physically, it addresses the important query: are there circumstances under which a given quantum state permits assignments of joint probabilities for the outcomes of a given set of incompatible observables [32,33]?

The quantum representative of $I_{S_i \bigcap S_j}$ is unique, and is just the symmetrised product of the projection operators [26,27]:

$$I_{S_i \bigcap S_j} \equiv I_{S_i} I_{S_j} \to \mathbf{\Pi}_{i\wedge j} \equiv \mathbf{\Pi}_{ij} = \frac{1}{2}(\pi_i \pi_j + \pi_j \pi_i). \quad (1)$$

The operator $\mathbf{\Pi}_{ij}$ in equation (1) is hermitian, but not a projection, unless $[\pi_i, \pi_j] = 0$. This is but the simplest example of the class of operators that we shall designate as pseudo projections. $\mathbf{\Pi}_{ij}$ possesses two important properties: (i) It has at least one negative eigenvalue (see, for example, [34]), and (ii) the set $\left\{\mathbf{\Pi}_{ij}\right\}$, of all pseudo projections corresponding to all possible joint outcomes of the two observables A, B, forms an over-complete set and yields a resolution of identity, as given by

$$\sum_i \sum_j \mathbf{\Pi}_{ij} = \sum_i \pi_i = \mathbf{1}; \sum_j \sum_i \mathbf{\Pi}_{ij} = \sum_j \pi_j = \mathbf{1}. \quad (2)$$

The proof is a direct consequence of completeness of eigen projections of each observable.

Pseudo-projections that represent an indicator function for joint outcomes of more than two observables are not unique. Of all the choices, we shall, for the present, employ the one obtained from Weyl ordering which is completely symmetric in all the projections. We then recover the expression introduced in [30]. Other inequivalent prescriptions have been discussed in Appendix A.

Pseudo projections with N observables also satisfy the following over completeness relation: let $\{\mathbf{\Pi}_{\{\alpha\}}^N\}$ be the set of all pseudo projections corresponding to all possible outcomes of the N observables at hand. The set $\{\alpha\}$ labels the outcomes of the observables. Let $\{\alpha\} = \{\beta, j\}$ where j labels to the outcome of the observable A^k and β collectively denotes the rest. Then,

$$\sum_j \mathbf{\Pi}_{\{\beta,j\}}^N = \mathbf{\Pi}_{\{\beta\}}^{N-1}. \quad (3)$$

As with $N = 2$, it is a direct consequence of the completeness of eigen projections of observables.

3.1 Pseudo probabilities and pseudo probability schemes

Pseudo projections generate pseudo probabilities. Let a system be in a state ρ. We then define the pseudo probability associated with a pseudo projection $\mathbf{\Pi}_{\{\alpha\}}^N$ to be

$$\mathcal{P}_{\{\alpha\}}^N = Tr\left\{\rho \mathbf{\Pi}_{\{\alpha\}}^N\right\}. \quad (4)$$

Since $\mathbf{\Pi}_{\{\alpha\}}^N$ can admit negative eigenvalues, the corresponding pseudo probability can also be negative. We shall designate the set of all pseudo probabilities generated by the set $\{\mathbf{\Pi}_{\{\alpha\}}^N\}$ – a pseudo probability scheme. By virtue of equation (2), it follows that pseudo probabilities in any scheme add up to one. As a consequence of equation (3), pseudo probability schemes for subsets of observables are just the marginals of the parent scheme. In particular, the marginal scheme with a commuting set of observables has probabilities predicted by quantum mechanics.

[1] More generally, it could be any sample space.

4 Pseudo projections that represent outcomes of any event

We observe that, in classical probability, the probability of any composite event, involving N observables, gets determined by the joint probability scheme for those N observables. By composite events we imply events that are composed of arbitrary combinations of conjunctions, disjunctions and negations (classical logical operations). Taking it as our guiding principle, we lay down the following definition for construction of the pseudo-projection that represents the outcome of any classical event:

Definition (D1): let $\mathcal{E}$ be any event consisting of combinations of outcomes of N distinct observables $A_1, A_2, \cdots, A_N$. The pseudo-projection representing the event can be obtained in three steps:

1. Identify the subset of probabilities $\{P_c^i, i = 1, 2, \cdots\}$ in the classical joint probability scheme (for outcomes of the N observables), the sum of which is the probability for the occurrence of the event $\mathcal{E}$; $P_c^{(\mathcal{E})} = \sum_i P_c^i$.
2. Let $\{\mathcal{P}_i; i = 1, 2, \cdots\}$ be the subset of corresponding pseudo probabilities in the associated pseudo probability scheme. Each of the classical joint probabilities in the RHS of the sum, $P_c^{(\mathcal{E})} = \sum_i P_c^i$, is then symbolically replaced by their corresponding pseudo-probabilities; $\mathcal{P}^{(\mathcal{E})} \equiv \sum_i \mathcal{P}_i$.
3. The pseudo projection that represents the event $\mathcal{E}$ is then obtained by replacing each pseudo-probability in the summation $\mathcal{P}^{(\mathcal{E})} \equiv \sum_i \mathcal{P}_i$ by its associated pseudo-projection, i.e., $\mathbf{\Pi}^{\mathcal{E}} \equiv \sum_i \mathbf{\Pi}_i$.

In short, the chain of mappings is as follows:

$$P_c^{(\mathcal{E})} \equiv \sum_i P_c^i \rightarrow \sum_i \mathcal{P}_i \rightarrow \sum_i \mathbf{\Pi}_i \equiv \mathbf{\Pi}^{\mathcal{E}}. \tag{5}$$

The following example illustrates the definition: the pseudo projection $\mathbf{\Pi}_{a\vee b}$ representing the indicator function, $I_{S_a \cup S_b}$, for the union of two overlapping supports S_a, S_b is given by the chain of mappings

$$\begin{aligned} P_c^{a\vee b} \;\; &\equiv \;\; \sum_{b'} P_c^{ab'} + \sum_{a'} P_c^{a'b} - P_c^{ab} \\ &\rightarrow \sum_{b'} \mathcal{P}_{ab'} + \sum_{a'} \mathcal{P}_{a'b} - \mathcal{P}_{ab} \\ &\rightarrow \pi_a + \pi_b - \mathbf{\Pi}_{ab} = \mathbf{\Pi}_{a\vee b}. \end{aligned} \tag{6}$$

5 Non-classicality of states

Definition (D2): let $\mathcal{S}_\rho(\{A^i; i = 1, \cdots, N\})$, be the pseudo probability scheme for a set of N observables, for a system in a state ρ. The state is non-classical with respect to these observables if, even one of the pseudo-probabilities in the scheme is negative. It may be deemed to be classical if, and only if, all the entries are non-negative.

If the pseudo-probability associated with an event assumes values outside [0, 1], it would serve as a signature of non classicality. Many designations of non-classicality, as for example done in, [3,5,35] belong to this category. In short, classicality of a state is relative and not absolute.

Suppose that all the entries in a pseudo-probability scheme are non-negative, even when the underlying projections are mutually non-commuting. It would mean, as it were, that the scheme represents joint probabilities for a correlated classical state, with quantum probabilities as its marginals.

Also, along the sidelines, the definition brings out the real import of the idea of negative probability advocated by Dirac, [36], Bartlett [37], and most forcefully, by Feynman [38]. It has been argued that the introduction of negative probability, even if it be in an *ad hoc* manner (as in p 11 of [38]), does have a role in the sense of consistent book keeping in intermediate processes (and calculations). This intuitive idea, set forth in [36,38], gets automatically incorporated in the present formalism. The smallest subset in the event space for which the pseudo-probability is not negative would give the minimum coarse graining required for a physical interpretation of joint probability. The relation of the present framework with violation of classical logic shown in [39] is discussed briefly in Appendix B.

6 Non-locality and entanglement in bipartite systems

This section presents the main applications of the formalism to bipartite systems. We are interested in the non-classicality residing in correlations between the two subsystems. For the purpose of this paper we shall consider two manifestations of non-classical correlations *viz.*, non-locality and entanglement.

In order to arrive at the conditions for these notions, in each case we choose pseudo-probabilities (for bipartite systems) such that:

1. Their sum involves two or more correlators between observables of the two subsystems. The observables of each subsystem do not share a common eigen-basis, e.g., if the sum involves two terms $\langle A_1 B_1 \rangle$ and $\langle A_2 B_2 \rangle$, where A_i, B_i are observables for first and second subsystem respectively, then, $[A_1, A_2] \neq 0$; $[B_1, B_2] \neq 0$.
2. In their sum, the contributions from local terms get cancelled.
3. The ensuing inequality is violated by all separable states, i.e., the sum of chosen pseudo-probabilities always lies in [0, 1] for all separable states.

Bell-CHSH non locality will be derived for any bipartite system. The entanglement inequalities are obtained only for two qubit systems.

6.1 Notations

First, we establish some notations for the sake of compactness. All observables, considered henceforth, are dichotomic, with eigenvalues ± 1. Thus, the two outcomes are negations of each other. The event $\mathcal{E}(A=+1)$ is denoted by $\mathcal{E}(A)$, and its negation, $\mathcal{E}(A=-1)$, by $\mathcal{E}(\overline{A})$. Joint outcomes are written as simple juxtapositions, by omitting the sign $\wedge$. We agree to separate observables belonging to different subsystems by a semicolon. The following example illustrates the notations.

$$\mathcal{E}\{A_1=+1\}\wedge\mathcal{E}\{B_1=-1\}\wedge\mathcal{E}\{B_2=+1\}\equiv\mathcal{E}\{A_1;\overline{B}_1B_2\}. \tag{7}$$

Here, the observables A_1 and $B_{1,2}$ belong to the first and the second subsystems respectively. The corresponding pseudo projection will be $\mathbf{\Pi}\{A_1;\overline{B}_1B_2\}=\pi_{A_1}\times\mathbf{\Pi}_{\overline{B}_1B_2}$ and the ensuing pseudo-probability will be denoted as $\mathcal{P}\{A_1;\overline{B}_1B_2\}$. Disjunction of events will be explicitly denoted by the standard symbol $\vee$.

6.2 Non-locality

Consider a $d_1\times d_2$ level system, and a pair of dichotomic observables, $A_{1,2}$ and $B_{1,2}$ respectively, for each subsystem. The underlying scheme $\mathcal{P}(A_1A_2;B_1B_2)$ consists of 16 entries. Of interest is the simplest of the non-trivial event involving incompatible observables, given by,

$$\begin{aligned}\mathcal{E}_{NL}\equiv\ &\mathcal{E}^1\{A_1;B_1B_2\}\vee\mathcal{E}^2\{\overline{A}_1;\overline{B}_1\overline{B}_2\}\\ &\vee\mathcal{E}^3\{A_2;B_1\overline{B}_2\}\vee\mathcal{E}^4\{\overline{A}_2;\overline{B}_1B_2\}.\end{aligned} \tag{8}$$

The quantum representative of the indicator function corresponding to the event $\mathcal{E}_{NL}$ shown in equation (8), following the definition **D1**, is the sum, $\mathbf{\Pi}_{NL}=\sum_i\mathbf{\Pi}_i$, of the pseudo projections representing each event $\mathcal{E}^i$. Note that none of the pseudo projections in the summand is a projection. A state ρ would be classical with respect to this event/ pseudo-projection if the corresponding pseudo-probability respects the bounds

$$0\le Tr\Big[\rho\mathbf{\Pi}_{NL}\Big]\le 1. \tag{9}$$

The identity, $\pi^A_{\pm 1}=\frac{1}{2}(\mathbf{1}\pm A)$, immediately leads to the classic Bell-CHSH inequality

$$\Big|\Big\langle A_1B_1+A_1B_2+A_2B_1-A_2B_2\Big\rangle_\rho\Big|\le 2. \tag{10}$$

This derivation throws light on the violation of the corresponding rule of classical probability in the form expressed in [5]. Truly, violation of Bell-CHSH inequality is autonomous of the kinematics of inertial frames. This observation does, by no means, diminish the deep physical and philosophical consequences that follow from combining non-locality with special relativity. The derivation also shows that jointly measurable observables cannot lead to the violation of the Bell-CHSH inequality [32,33,40,41]. It will be seen that this last conclusion continues to hold true for entanglement also.

For future comparison, we recast equation (10) for the two-qubit case in terms of correlations, for the special geometry $\hat{a}_1\cdot\hat{a}_2=\hat{b}_1\cdot\hat{b}_2=0$. We employ the forms $A_{1,2}=\boldsymbol{\sigma}\cdot\hat{a}_{1,2}$ and $B_{1,2}=\mathbf{\Sigma}\cdot\hat{b}_{1,2}$ in terms of the Pauli bases in the respective subspaces. Writing the normalised sum of vectors as $\hat{b}=\frac{1}{\sqrt{2}}(\hat{b}_1+\hat{b}_2)$ and $\hat{b}'=\frac{1}{\sqrt{2}}(\hat{b}_1-\hat{b}_2)$, we obtain the following inequality for non-locality,

$$\Big|\Big\langle\boldsymbol{\sigma}\cdot\hat{a}_1\mathbf{\Sigma}\cdot\hat{b}+\boldsymbol{\sigma}\cdot\hat{a}_2\mathbf{\Sigma}\cdot\hat{b}'\Big\rangle\Big|>\sqrt{2}. \tag{11}$$

6.3 Entanglement

Though all non-local states are entangled, the converse statement is not necessarily true [6], suggesting that entanglement admits further refinements. Further, settling whether a state is entangled or not is a hard problem, which has led to several more modest approaches such as majorisation relations, conditions based on correlation tensors and studies involving concurrence [42–44]. Rather than hunt for a single combination of pseudo-probability that would deliver an inequality which is capable of detecting all entangled states, we take up two-qubit systems, and systematically propose (a) two events from which conditions of entanglement follow as violation of rules of classical probability (b) direct combinations of pseudo-probabilities (without averring to the underlying events, which can be rather complicated) which also renders a set of entanglement inequalities arising from violations of classical probability rules.

6.3.1 Entanglement inequalities from explicit events

Event 1

As usual, A stands for the observable $\boldsymbol{\sigma}\cdot\hat{a}$. Henceforth, we denote the observables in the first and the second subsystems respectively by Latin and Greek symbols. The respective Pauli operators will be denoted by σ_i and Σ_i. The first event has the same number of observables as in non locality, only with additional constraints, leading to further identification of non-classical states. Thus, in the two doublets of observables, $\{A_1,A_2\}$ and $\{\Phi_1,\Phi_2\}$ for the first and second qubit respectively, we impose the orthogonality conditions $\hat{a}_1\cdot\hat{a}_2=\hat{\phi}_1\cdot\hat{\phi}_2=0$. Furthermore, the event of interest is shown below:

$$\begin{aligned}&\mathcal{E}^1\{A_1A_2;\Phi_1\Phi_2\}\vee\mathcal{E}^2\{\overline{A}_1\overline{A}_2;\overline{\Phi}_1\overline{\Phi}_2\}\\ &\vee\mathcal{E}^3\{A_1\overline{A}_2;\Phi_1\overline{\Phi}_2\}\vee\mathcal{E}^4\{\overline{A}_1A_2;\overline{\Phi}_1\Phi_2\}.\end{aligned} \tag{12}$$

Following definition **D1** for construction of quantum representative for the event shown in equation (12) and demanding the ensuing pseudo probability to be negative, we arrive at the first sufficiency condition for entanglement given by

$$\Big\langle\boldsymbol{\sigma}\cdot\hat{a}_1\mathbf{\Sigma}\cdot\hat{\phi}_1+\boldsymbol{\sigma}\cdot\hat{a}_2\mathbf{\Sigma}\cdot\hat{\phi}_2\Big\rangle<-1. \tag{13}$$

The correlations in equation (13) are the same as in equation (11). The new bound renders more states non-classical, restating the fact that there are entangled states which are local. This distinction raises the possibility that inclusion of more observables (classical joint observations) may lead to even better entanglement inequalities.

Event 2

We now consider two triplets each of three orthogonal observables, $\{A_i\}, \{\Phi_i\}; i \in \{1, 2, 3\}$ for the first and second qubit respectively. The pseudo-probability scheme $\mathcal{P}(A_1 A_2 A_3; \Phi_1 \Phi_2 \Phi_3)$ would consist of 2^6 entries. But for our purposes, it suffices to examine the following composite event:

$$\begin{aligned} &\mathcal{E}^1\{A_1 A_2 A_3; \Phi_1 \Phi_2 \Phi_3\} \vee \mathcal{E}^2\{\overline{A}_1 \overline{A}_2 \overline{A}_3; \overline{\Phi}_1 \overline{\Phi}_2 \overline{\Phi}_3\} \\ &\quad \vee \mathcal{E}^3\{\overline{A}_1 A_2 A_3; \overline{\Phi}_1 \Phi_2 \Phi_3\} \vee \mathcal{E}^4\{A_1 \overline{A}_2 \overline{A}_3; \Phi_1 \overline{\Phi}_2 \overline{\Phi}_3\} \\ &\quad \vee \mathcal{E}^5\{A_1 \overline{A}_2 A_3; \Phi_1 \overline{\Phi}_2 \Phi_3\} \vee \mathcal{E}^6\{\overline{A}_1 A_2 \overline{A}_3; \overline{\Phi}_1 \Phi_2 \overline{\Phi}_3\} \\ &\quad \vee \mathcal{E}^7\{A_1 A_2 \overline{A}_3; \Phi_1 \Phi_2 \overline{\Phi}_3\} \vee \mathcal{E}^8\{\overline{A}_1 \overline{A}_2 A_3; \overline{\Phi}_1 \overline{\Phi}_2 \Phi_3\}. \end{aligned} \tag{14}$$

Yet again, following **D1**, the pseudo projection for the event is simply the sum of various pseudo projections for individual events. Violation of non negativity requirement for the associated pseudo probability yields the following inequality for a state to be entangled:

$$\left\langle \boldsymbol{\sigma} \cdot \hat{a}_1 \boldsymbol{\Sigma} \cdot \hat{\phi}_1 + \boldsymbol{\sigma} \cdot \hat{a}_2 \boldsymbol{\Sigma} \cdot \hat{\phi}_2 + \boldsymbol{\sigma} \cdot \hat{a}_3 \boldsymbol{\Sigma} \cdot \hat{\phi}_3 \right\rangle < -1. \tag{15}$$

The inequality (15) is not new, and has been derived earlier by Gühne et al. [35] and Werner [6]. We note that their derivation is driven by purely algebraic considerations, in contrast to our approach which is motivated by violations of classical rules of probability. An even more direct derivation will be given in Section 6.3.2. We emphasize that the pseudo-probabilities contributing to the events in (8), (12) and (14) conform to the rules laid down in Section 6.

6.3.2 Entanglement inequalities from direct combinations of pseudo-probabilities from a scheme

In this section, we look at sums of such entries from a pseudo-probability scheme and their marginals that lead to violations of classical probability thereby yielding conditions for entanglement.

Inequality 1

First, we consider a pair of mutually orthogonal observables A_1, A_2 for the first qubit and two triplets of mutually orthogonal observables $\{\Phi_1, \Phi_2, \Phi_3\}, \{\Theta_1, \Theta_2, \Theta_3\}$ for the second. To specify the detector geometry completely, the normalised sums of the vectors, in the respective triplets $\{\Phi_i\}$ and $\{\Theta_i\}$, given by $\hat{\phi} = \sum_{i=1}^{3} \hat{\phi}_i/\sqrt{3}$ and $\hat{\theta} = \sum_{i=1}^{3} \hat{\theta}_i/\sqrt{3}$, are chosen to be orthogonal: $\hat{\phi} \cdot \hat{\theta} = 0$. The number of pseudo probabilities is 2^8. But we may look at the sum of the marginals

$$\begin{aligned} \mathcal{P}_{E_1} &= \mathcal{P}\{A_1; \Phi_1 \Phi_2 \Phi_3\} + \mathcal{P}\{\overline{A}_1; \overline{\Phi}_1 \overline{\Phi}_2 \overline{\Phi}_3\} \\ &\quad + \mathcal{P}\{A_2; \Theta_1 \Theta_2 \Theta_3\} + \mathcal{P}\{\overline{A}_2; \overline{\Theta}_1 \overline{\Theta}_2 \overline{\Theta}_3\} \end{aligned} \tag{16}$$

and demand it to be negative. We arrive at a sufficiency condition for entanglement given by

$$\left\langle \boldsymbol{\sigma} \cdot \hat{a}_1 \boldsymbol{\Sigma} \cdot \hat{\phi} + \boldsymbol{\sigma} \cdot \hat{a}_2 \boldsymbol{\Sigma} \cdot \hat{\theta} \right\rangle < -\frac{2}{\sqrt{3}}. \tag{17}$$

Inequality 2

The next inequality may be derived by enlarging the scheme further. For the first subsystem, we consider three sets of doublets $\{A_i\}$, $\{B_i\}$, $\{C_i\}$ where observables within each set are mutually orthogonal. For the second (sub)system, we choose three sets of triplets $\{\Phi_i\}, \{\Theta_i\}, \{\Psi_i\}$ where again, each triplet consists of mutually orthonormal observables. As in the earlier cases, the detector geometry is specified by requiring that both the sets of normalised sums $\left\{\hat{a}, \hat{b}, \hat{c}\right\}$ and $\left\{\hat{\phi}, \hat{\theta}, \hat{\psi}\right\}$ be orthonormal sets. The sum of marginals of interest is

$$\begin{aligned} \mathcal{P}_{E_2} &= \mathcal{P}\{A_1 A_2; \Phi_1 \Phi_2 \Phi_3\} + \mathcal{P}\{\overline{A}_1 \overline{A}_2; \overline{\Phi}_1 \overline{\Phi}_2 \overline{\Phi}_3\} \\ &\quad + \mathcal{P}\{B_1 B_2; \Theta_1 \Theta_2 \Theta_3\} + \mathcal{P}\{\overline{B}_1 \overline{B}_2; \overline{\Theta}_1 \overline{\Theta}_2 \overline{\Theta}_3\} \\ &\quad + \mathcal{P}\{C_1 C_2; \Psi_1 \Psi_2 \Psi_3\} + \mathcal{P}\{\overline{C}_1 \overline{C}_2; \overline{\Psi}_1 \overline{\Psi}_2 \overline{\Psi}_3\} \end{aligned} \tag{18}$$

which leads to an independent sufficiency condition, i.e., a new entanglement inequality for non-separability, which has the form

$$\left\langle \boldsymbol{\sigma} \cdot \hat{a} \boldsymbol{\Sigma} \cdot \hat{\phi} + \boldsymbol{\sigma} \cdot \hat{b} \boldsymbol{\Sigma} \cdot \hat{\theta} + \boldsymbol{\sigma} \cdot \hat{c} \boldsymbol{\Sigma} \cdot \hat{\psi} \right\rangle < -\sqrt{\frac{3}{2}}. \tag{19}$$

Inequality 3

Finally, we consider three triplets of mutually orthogonal observables $\{A_i\}, \{B_i\}, \{C_i\}$ for the first qubit, and another set of three triplets of orthogonal observables $\{\Phi_i\}, \{\Theta_i\}, \{\Psi_i\}$ for the second. As before, the normalised sums are chosen to be mutually orthogonal for each qubit. The sum of the marginals of pseudo probabilities, which is more involved, is displayed below:

$$\begin{aligned} \mathcal{P}_{E_3} &= \mathcal{P}\{A_1 A_2 A_3; \Phi_1 \Phi_2 \Phi_3\} + \mathcal{P}\{\overline{A}_1 \overline{A}_2 \overline{A}_3; \overline{\Phi}_1 \overline{\Phi}_2 \overline{\Phi}_3\} \\ &\quad + \mathcal{P}\{B_1 B_2 B_3; \Theta_1 \Theta_2 \Theta_3\} + \mathcal{P}\{\overline{B}_1 \overline{B}_2 \overline{B}_3; \overline{\Theta}_1 \overline{\Theta}_2 \overline{\Theta}_3\} \\ &\quad + \mathcal{P}\{C_1 C_2 C_3; \Psi_1 \Psi_2 \Psi_3\} + \mathcal{P}\{\overline{C}_1 \overline{C}_2 \overline{C}_3; \overline{\Psi}_1 \overline{\Psi}_2 \overline{\Psi}_3\}. \end{aligned} \tag{20}$$

Classicality would force $\mathcal{P}_{E_3}$ to be non-negative. Its violation yields an improved sufficiency condition for entanglement, given by

$$\left\langle \boldsymbol{\sigma} \cdot \hat{a} \boldsymbol{\Sigma} \cdot \hat{\phi} + \boldsymbol{\sigma} \cdot \hat{b} \boldsymbol{\Sigma} \cdot \hat{\theta} + \boldsymbol{\sigma} \cdot \hat{c} \boldsymbol{\Sigma} \cdot \hat{\psi} \right\rangle < -1.$$

This inequality is the same as equation (15).

More pertinently, this analysis shows that none of these non-classicality conditions would follow if all the entries in the underlying pseudo-probability scheme were non-negative. A seemingly similar approach employed in [45] does not yield entanglement inequalities since a prior knowledge of the state is assumed to determine if the state is entangled. In [46], the negative value assumed by a linear combination of pseudoprobabilities (different from the ones for the event given in equation (8)) has been used to show violation of Bell inequality only for pure two qubit and two qutrit systems.

Just as with the distinction between non-locality and entanglement, the inequalities derived in this section induce a further refinement in characterising entanglement, depending on the set of classical rules violated by the states. We explore their interrelationship in greater detail in the next section.

7 Examples and discussion

We label the five inequalities for entanglement, 11, 17, 13, 19 and 15 as $\mathbf{W_0}, \mathbf{W_1}, \mathbf{W_2}, \mathbf{W_3}$ and $\mathbf{W_4}$ respectively. The operator in the LHS of the inequality $\mathbf{W}_i$ shall be denoted as $\mathbf{O}_i$. For illustration and further discussion, we shall begin with the special class of states, obtained by the addition of a local term to the Werner states,

$$\rho = \frac{1}{4}(\mathbf{1} + \alpha\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} + \beta\sigma_z). \tag{21}$$

The main results are captured in Figure 1a. The region bounded by the points A, B, C and D, represents the space of all allowed states. The line AC represents the Werner states, and the region contained between the arcs BED and BCD corresponds to separable states. The vertex A represents the fully entangled singlet state, and the point O, the completely mixed state.

The five vertical lines mark the boundaries of sets of entangled states (triangles with A as their common vertex) detected by respective inequalities. Of them, the first line L_0 marks the boundary between non-local and local states. The subsequent lines represent, in order, the sets of entangled states detected by the set of four sufficiency conditions, $\mathbf{W_i}$, in the same order. The last line, L_4 encompasses the largest region, which includes all the entangled Werner states. But it is still not exhaustive since it fails to detect entangled states in the region shaded in pink. The existence of a such a combination of pseudo-probability leading to an entanglement inequality that detects all the entangled state is yet to be demonstrated.

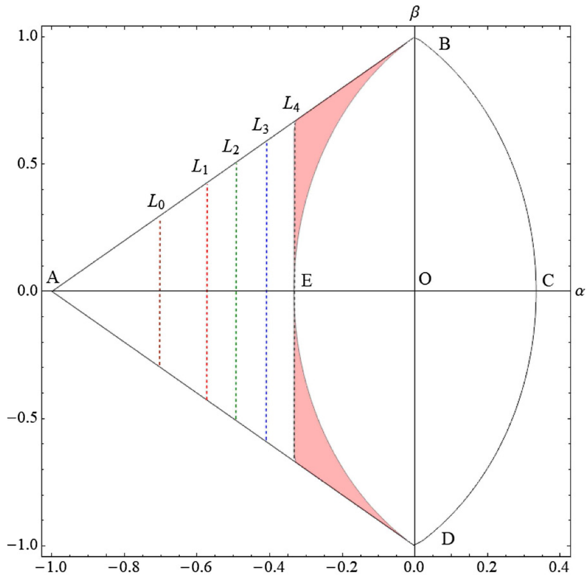
It is possible to draw several stronger conclusions for more general states. Consider an arbitrary two-qubit state in the SVD basis,

$$\rho = \frac{1}{4}(\mathbf{1} + \mathbf{P}\cdot\boldsymbol{\sigma} + \mathbf{Q}\cdot\boldsymbol{\Sigma} + \sum_{i=1}^{3} t_i\sigma_i\Sigma_i). \tag{22}$$

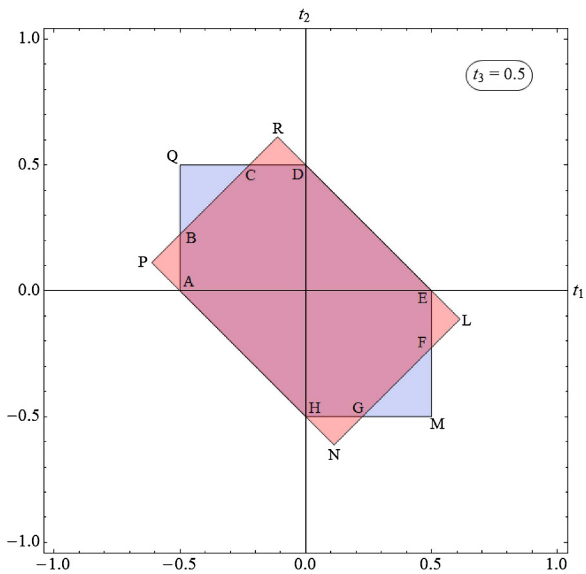
The entanglement inequalities, comprising entirely of correlations, are sensitive only to the singular values t_i. Each inequality, therefore detects entangled states in regions, determined by the corresponding set of inequalities imposed on the singular values. The region of the correlation space that represents a state is a tetrahedron, defined by the four bounds [47],

$$\begin{aligned} &1 - t_1 - t_2 - t_3 \geq 0\ ;\ 1 - t_1 + t_2 + t_3 \geq 0 \\ &1 + t_1 - t_2 + t_3 \geq 0\ ;\ 1 + t_1 + t_2 - t_3 \geq 0. \end{aligned} \tag{23}$$

First consider the inequality $\mathbf{W_4}$. It partitions the correlation space into two parts. States that are separable



(a)



(b)

Fig. 1. (a)Figure showing the relative strengths of the entanglement inequalities in the parameter space of $\rho = \frac{1}{4}(\mathbf{1} + \alpha\boldsymbol{\sigma}\cdot\boldsymbol{\Sigma} + \beta\sigma_z)$. See text for details. (b)PRLN: projection of R_1 on (t_1, t_2) plane with $t_3 = 0.5$. AQDEMHA: projection of R_2 on (t_1, t_2) plane with $t_3 = 0.5$. See text for details.

and those that are entangled but evade detection by $\mathbf{W_4}$, satisfy the conditions:

$$\begin{aligned} &1 + t_1 + t_2 + t_3 \geq 0\ ;\ 1 + t_1 - t_2 - t_3 \geq 0 \\ &1 - t_1 + t_2 - t_3 \geq 0\ ;\ 1 - t_1 - t_2 + t_3 \geq 0. \end{aligned} \tag{24}$$

The first condition follows from the inequality $\mathbf{W_4}$ for the configuration $\hat{a}_1 = \hat{\phi}_1 = \hat{x}; \hat{a}_2 = \hat{\phi}_2 = \hat{y}; \hat{a}_3 = \hat{\phi}_3 = \hat{z}$. The second, third and fourth conditions follow from $\mathrm{Tr}\{((\sigma_i \times \mathbf{1})\mathbf{O}_4(\sigma_i \times \mathbf{1}))\rho\} \geq 0; (i \in \{1, 2, 3\})$ respectively, keeping the configuration intact. Together with conditions in equation (23), they constitute the interior (and surface) of an octahedron.

The complementary region lying outside the octahedron corresponds to the entangled states detected by $\mathbf{W_4}$. This sufficiency condition also becomes necessary for the Bell diagonal states, as may be seen by employing partial transpose criterion, and as also displayed in Figure 1a for the special case of Werner states.

Thus, for the Bell diagonal states $\mathbf{W_4}$ is the strongest. But it still leaves the relative strengths of the four inequalities undetermined. To settle that we shall consider the other three inequalities. Starting with $\mathbf{W_3}$ we arrive at a new set of conditions:

$$\sqrt{\frac{3}{2}}+t_1+t_2+t_3\geq 0\ ;\ \sqrt{\frac{3}{2}}+t_1-t_2-t_3\geq 0$$
$$\sqrt{\frac{3}{2}}-t_1+t_2-t_3\geq 0\ ;\ \sqrt{\frac{3}{2}}-t_1-t_2+t_3\geq 0 \quad (25)$$

which, together with equation (23) define a larger octahedron R_1, which contains the separable and (undetected) entangled states[2]. As before, (t_1,t_2,t_3) corresponding to the entangled states detected by $\mathbf{W_3}$ must lie outside the octahedron. Between $\mathbf{W_4}$ and $\mathbf{W_3}$, the former is, of course, stronger. Of real interest, however, is to compare them with the conditions obtained by $\mathbf{W_{1,2}}$. These yield two sets of 12 bounds (that define the dodecahedron),

$$c\pm t_1\pm t_2\geq 0; c\pm t_2\pm t_3\geq 0; c\pm t_3\pm t_1\geq 0 \quad (26)$$

with $c=\frac{2}{\sqrt{3}}(1)$ for $\mathbf{W_1}(\mathbf{W_2})$[3]. Two sets of these 12 conditions corresponding to $c=\frac{2}{\sqrt{3}}$ and $c=1$, in conjunction with equation (23), yield the required region in the correlation space, that contains all the separable states and also some (undetected) entangled states by $\mathbf{W}_1$ and $\mathbf{W}_2$ respectively. We label the region obtained corresponding to $c=1$ as R_2. The states lying outside the respective regions are all entangled and get detected.

With the regions thus identified, we may immediately conclude that $\mathbf{W_4}$ is the strongest and that $\mathbf{W_3}$ is stronger than $\mathbf{W_1}$. We already know that $\mathbf{W_2}$ is stronger than $\mathbf{W_1}$. However, as may be seen in Figure 1b, $\mathbf{W_2}$ and $\mathbf{W_3}$ are mutually independent, since the entangled states that are detected have only partial overlaps. In Figure 1b we show the projection of R_1 and R_2 in (t_1,t_2) plane, with $t_3=0.5$. The hexagon $QDEMHA$ and the rectangle $PRLN$ constitute the set of separable and undetected entangled states for $\mathbf{W_2}$ and $\mathbf{W_3}$, respectively. The overlap is the octagon $ABCDEFGH$. The triangles QBC and MGF are detected only by $\mathbf{W_3}$. Likewise the triangles CDR, EFL, GHN, ABP are detected only by $\mathbf{W_2}$. These results, together with the examples discussed, reinforce the statement that different inequalities reflect substructures in the space of entangled states that arise from violations of different classical rules.

8 Conclusion

This paper employs a quantitative framework for quantum probability to develop the notion of pseudo-projections. Pseudo projection operators, representing probabilities for classical events, are shown to reveal non classicality of states in myriad forms. The power of the method is illustrated by employing elementary methods to recover the famous Bell-CHSH inequality and sufficiency conditions on entanglement, without recourse to purely algebraic techniques. Conceptually, this study brings out the unity underlying negative probability [36–38], and criteria for non-classicality [3,5,7,11]. Thus, it opens up a fertile field for a systematic theoretical and experimental investigation of many more tests of non-classicality of states.

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Author contribution statement

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Appendix A: Inequivalent quantum representatives for joint outcomes of multiple observables

When the number of observables N exceeds two, the representative pseudo projections for their joint outcomes are not unique. Consider a joint event involving outcomes of N observables $\left\{A^k=a^k_{i_k}; k=1,2,\cdots,N\right\}$, where the index k labels the observable. If we were to denote the product of the corresponding projection operators in some order – collectively denoted by the ordered set $\{q\}$ – by $\mathcal{A}^N_{\{q\}}$, then the hermitised sum

$$\mathbf{\Pi}^N_{\{q\}}=\frac{1}{2}(\mathcal{A}^N_{\{q\}}+\mathcal{A}^{N\dagger}_{\{q\}}) \quad (A.1)$$

serves as a valid quantum representative of the corresponding classical indicator function, i.e., it is a pseudo projection. We call this a unit pseudo projection. There are $\frac{N!}{2}$ such unit pseudo projections, depending on the order in which the projection operators are arranged. The representative pseudo projection can be chosen to be any element in the manifold which is the convex span of these unit pseudo projections. In general, each element in the

[2] The first condition in equation (25)can be arrived at by choosing $\hat{a}=\hat{\phi}=\hat{x};\hat{b}=\hat{\theta}=\hat{y};\hat{c}=\hat{\psi}=\hat{z}$. The remaining conditions can be obtained by demanding $\mathrm{Tr}\{((\sigma_i\times\mathbf{1})\mathbf{O}_3(\sigma_i\times\mathbf{1}))\rho\}\geq 0; (i\in\{1,2,3\})$ for the same configuration.

[3] The conditions $c\pm t_1\pm t_2\geq 0$ is emergent after choosing $\hat{a}_1=\hat{\phi}=\pm\hat{x};\hat{a}_2=\hat{\theta}=\pm\hat{y}$ for $\mathbf{W}_1$ and $\hat{a}_1=\hat{\phi}_1=\pm\hat{x};\hat{a}_2=\hat{\phi}_2=\pm\hat{y}$ for $\mathbf{W}_2$. The other sets of inequalities emerge by changing $\{\hat{x},\hat{y},\hat{z}\}$ cyclically.

convex span yields an inequivalent quantum representative of the underlying indicator function. The manifold would collapse to a single point if all the projections were to commute.

Appendix B: Differences with classical logic

In this appendix, we briefly discuss how quantum logic deviates from the classical formulation. First of all, consider pseudo projections. Non-classical logic, as understood in [39], is inherent in the very definition of pseudo projections. The formalism developed in [39] identifies joint outcomes of non-commuting observables with absurd propositions in the quantum domain, although they are perfectly valid classically. The violations of Boolean logic, that they aver, arise from this identification. The present work does capture this qualitative observation more sharply and quantitatively, through the emergence of negative eigenvalue(s) of the corresponding pseudo projections.

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