Discord of bipartite correlations in generalized nonsignaling theories and its implications to quantum correlations

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We introduce the measures, Bell discord (BD) and Mermin discord (MD), for investigating bipartite nonsignaling (NS) correlations. These measures divide the nonsignaling polytope into four regions which have (i) nonzero BD and zero MD, (ii) zero BD and nonzero MD, (iii) nonzero BD and nonzero MD, and (iv) zero BD and zero MD. We show that any NS correlation can be written as the convex mixture of a PR-box, a maximal Mermin discordant box, and a Bell local box which has zero BD and zero MD. We show that BD and MD quantify nonclassicality of all quantum-quantum states, which are neither classical-quantum states nor quantum-classical states, for all incompatible measurements.

I. INTRODUCTION

Bell showed that measurements on spatially separated entangled system can lead to nonlocal correlations which cannot be explained by local hidden variable (LHV) theory [1]. Nonlocality is witnessed by the violation of a Bell inequality which puts upper bound on the correlations under the constraint of the LHV theory. Nonlocality is not the unique nonclassical feature of quantum theory as nonquantum correlations, which cannot be used for instantaneous signaling, can also violate Bell inequality. Further, nonlocality of quantum theory is limited by Tsirelson bound [2]. Popescu and Rohrlich showed that the limited violation of Bell inequality by quantum theory is not a consequence of relativity [3].

In generalized nonsignaling theory (GNST), the correlations are constrained only by the nonsignaling principle [4]. Quantum theory is a subclass of a GNST that achieves maximal nonlocality. One of the goal for studying GNST is to find out what singles out quantum thoery from other nonsignaling theories [5]. Quantum key distribution was studied in the context of GNST in which nonlocality is responsible for security [6].

In this work, we introduce two measures, Bell discord and Mermin discord, to investigate quantum correlations in the framework of GNST. The set of nonsignaling correlations forms a convex polytope which can be divided into nonlocal region and local polytope. The quantum correlations forms a subset of NS polytope which allows to decompose quantum correlations as the convex combination of the extremal boxes of the polytope. Bell local correlations, which are considered as classical correlations, can have Bell discord or Mermin discord. The extremal nonclassical correlations with respect to Bell discord are the extremal nonlocal boxes, whereas the extremal nonclassical correlations with respect to Mermin discord lie inside the local polytope. We study the decomposition of any NS correlation with respect to these measures. Nonlocality of quantum correlations implies that the correlations are obtained when incompatible measurements are performed on the entangled states. Not all entangled states can lead to nonlocality even when incompatible measurements are performed on them. We show that the correlations arising from all the quantum-quantum states can have nonzero Bell discord or Mermin discord or both of them together when incompatible measurements are performed on them.

The paper is organized as follows. In Sec. II, we introduce the bipartite Bell-CHSH scenario with two-inputs and two-outputs and we discuss the motivations for defining nonclassicality for Bell local correlations. In Sec. III, we review the geometry of bipartite nonsignaling boxes. In Sec. IV, we introduce Bell discord and Mermin discord. In sec. V, we investigate quantum correlations in Schmidt states, Werner states, mixture of maximally entangled state with classically correlated state, and classical-quantum states and quantum-classical states using these measures. Conclusions are provided in Sec. VI.

II. PRELIMINARIES

Consider Bell-CHSH scenario [8] in which two spatially separated parties make two dichotomic measurements on their respective subsystems, the correlations between the outcomes is described by the joint probability distribution (JPD),

$$P(a_m,b_n|A_i,B_j) = \begin{vmatrix} P(a_0,b_0|A_0,B_0) & P(a_0,b_1|A_0,B_0) & P(a_1,b_0|A_0,B_0) & P(a_1,b_1|A_0,B_0) \\ P(a_0,b_0|A_1,B_0) & P(a_0,b_1|A_1,B_0) & P(a_1,b_0|A_1,B_0) & P(a_1,b_1|A_1,B_0) \\ P(a_0,b_0|A_0,B_1) & P(a_0,b_1|A_0,B_1) & P(a_1,b_0|A_0,B_1) & P(a_1,b_1|A_0,B_1) \\ P(a_0,b_0|A_1,B_1) & P(a_0,b_1|A_1,B_1) & P(a_1,b_0|A_1,B_1) & P(a_1,b_1|A_1,B_1) \end{vmatrix}.$$ (1)
In lab, Alice and Bob estimate $P(a_m, b_n | A_i, B_j)$ by making von Neum man measurements on an ensemble of bipar tite two-qubit systems described by the density matrix $\rho_{AB}$ in the Hilbert space $H^A \otimes H^B$. Quantum theory predicts the correlations through the Born’s rule, $P(a_m, b_n | A_i, B_j) = \text{Tr} (\Pi^a_m \otimes \Pi^b_n | A_i, B_j)$, where $\Pi^a_m = 1/2 (I + a_m \hat{a} \cdot \vec{\sigma})$ and $\Pi^b_n = 1/2 (I + b_n \hat{b} \cdot \vec{\sigma})$, are the projectors generating binary outcomes $a_m, b_n \in \{-1, 1\}$. Since quantum correlation arises from the tensor product structure, by definition it is nonsignaling; that is the marginal distribution of Alice is independent from the tensor product structure, by definition it is nonsignaling.

For instance, the Bell state, a maximally entangled state can be locally contextual in two-qubit systems described by the density matrix $\rho_{AB} = \frac{1}{2} (|00\rangle + |11\rangle) \otimes \gamma$ with $\gamma = \sqrt{p} |0\rangle + \sqrt{1-p} |1\rangle$, achieves Tsirelson bound can be written as the convex mixture of the PR-box and white noise:

$$P_{PR} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix},$$

and violates the Bell-CHSH inequality to its algebraic maximum, $B = 4$. Maximal quantum nonlocality can be achieved by making measurements on a maximally entangled system. For instance, the Bell state, $|\psi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$, gives rise to $B = 2 \sqrt{2}$, for the measurement observables: $A_0 = \sigma_x, A_1 = \sigma_y, B_0 = \frac{1}{\sqrt{2}} (\sigma_x - \sigma_y)$ and $B_1 = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_y)$. The JPD that achieves Tsirelson bound can be written as the convex mixture of the PR-box and white noise:

$$P = pP_{PR} + (1-p)P_N,$$

with $p = \frac{1}{\sqrt{2}}$. This representation of maximal quantum nonlocality in GNST motivates us to define a new nonclassicality for any correlations which has nonzero fraction of irreducible PR-box. We call this nonclassicality Bell discord which is weaker than Bell nonlocality in that Bell local correlations also violate the Bell-CHSH inequality to its algebraic maximum.

Quantum correlations can have nonzero components of irreducible PR-box and irreducible Mermin box simultaneously. For the measurements: $A_0 = \sigma_x, A_1 = \sigma_y, B_0 = \sqrt{p} \sigma_x - \sqrt{1-p} \sigma_y$ and $B_1 = \sqrt{1-p} \sigma_x + \sqrt{p} \sigma_y$, where $0 \leq p \leq \frac{1}{2}$, the Bell state gives rise to the following decomposition,

$$P = G^\prime P_{PR} + Q^\prime P_M + (1 - G^\prime - Q^\prime)P_N,$$

where $G^\prime = \frac{1}{\sqrt{2}} |\sqrt{p} + \sqrt{1-p}|$ and $Q^\prime = |\sqrt{p} - \sqrt{1-p}|$.

**III. POLYTOPE OF NONSIGNALING BOXES**

Barrett et al. [4] showed that the set of nonsignaling boxes (N) with two-inputs and two-outputs forms an 8 dimensional convex polytope which has 24 vertices. The vertices (or extremal boxes) of this polytope are 8 PR-boxes,

$$P^{\text{PR}}_{AB} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix},$$

and 16 deterministic boxes:

$$P^{\text{D}}_{AB} = \begin{pmatrix} 1, & m = \alpha \oplus \beta \\ n = \gamma \oplus \epsilon \\ 0, \end{pmatrix}$$

for the measurement observables, $A_0 = \sigma_x, A_1 = \sigma_y, B_0 = \sigma_x$ and $B_1 = -\sigma_y$. The above box does not violate a Bell-CHSH inequality, yet it is nonclassical in the sense that it does not admit a non-contextual-realistic value assignment: The first and fourth rows in Eq. (5) imply that the outcomes of $A_0B_0 = A_1B_1 = 1$. If the outcomes are predetermined, it should satisfy, $A_0B_1B_0 = 1$, but this contradicts the rows 2 and 3 because there is a nonzero probability for $A_0B_1 = -1$ and $A_1B_0 = 1$ and vice versa. The Mermin box also has contextuality argument in quantum theory since the state is simultaneous eigenstate of the observables, $\sigma_x \otimes \sigma_z, \sigma_y \otimes \sigma_z$ and $\sigma_x \otimes \sigma_y, (\sigma_x \otimes \sigma_y) (\sigma_y \otimes \sigma_x) = -\sigma_x \otimes \sigma_z$, i.e.,

$$\langle \sigma_x \otimes \sigma_z | \rho^+ \rangle = \langle \sigma^+ \rangle$$

$$\langle \sigma_y \otimes \sigma_z | \rho^- \rangle = -\langle \sigma^- \rangle$$

The above relation gives contextuality proof as shown by Peres in (10). Furthermore, the box violates the EPR-steering inequality [11].

$$\langle A_0 \sigma_x \rangle + \langle A_1 \sigma_y \rangle \leq \sqrt{2},$$

maximally. For this choice of observables, the correlation obtained by the nonmaximally entangled state $|\psi(\theta)\rangle = \cos \theta |00\rangle + \sin \theta |11\rangle$ can be written as,

$$P = pP_M + (1-p)P_N,$$
Here \(\alpha, \beta, \gamma, \epsilon \in [0, 1]\) and \(\otimes\) denotes addition modulo 2. Any NS correlation can be written as the convex sum of the 24 extremal boxes:

\[
P(a_m, b_n|A_i, B_j) = \sum_{k=0}^{7} p_k P_{PR}^k + \sum_{l=0}^{15} q_l P_D^l; \sum_k p_k + \sum_l q_l = 1,
\]

(12)

here \(k = \alpha\beta\gamma\) and \(l = \alpha\beta\gamma\epsilon\). All the deterministic boxes can be written as the product of marginals corresponding to Alice and Bob, \(P_D(a_m, b_n|A_i, B_j) = P_D(a_m|A_i)P_D(b_n|B_j)\), whereas the 8 PR-boxes cannot be written in the product form. Note that unlike the deterministic boxes, the marginals of the PR boxes are maximally mixed: i.e., \(P(a_m|A_i) = \frac{1}{2} = P(b_n|B_j)\) for all \(i, j, m, n\). The extremal boxes in a given class are related to each other through local reversible operations (LRO). A LRO simply relabels the inputs and outputs such that the class of the vertices remain invariant: Alice changing her input \(i \to i'\) and changing her output conditioned on the input: \(m \to m'\) or \(a_i \to \beta\). Bob can perform similar operations. A LRO thus converts a deterministic box into another deterministic box, a PR box into another PR box.

Bell polytope (\(\mathcal{L}\)), which is a subpolytope of \(\mathcal{N}\), is a convex hull of the 16 deterministic boxes: if \(P(a_m, b_n|A_i, B_j) \in \mathcal{L}\),

\[
P(a_m, b_n|A_i, B_j) = \sum_{l=0}^{15} q_l P_D^l; \sum_l q_l = 1.
\]

(13)

Fine [12] showed that the necessary and sufficient condition for the local deterministic strategy given in Eq. (13) is the complete set of Bell-CHSH inequalities:

\[
\mathcal{B}_{\alpha\beta\gamma} := (-1)^\gamma \langle A_0 B_0 \rangle + (-1)^{\beta\gamma} \langle A_0 B_1 \rangle
+ (-1)^{\beta\gamma} \langle A_1 B_0 \rangle + (-1)^{\alpha\beta\gamma\epsilon} \langle A_1 B_1 \rangle \leq 2,
\]

(14)

which are the nontrivial facets of the Bell polytope. All non-local correlations lie outside the Bell polytope and violate a Bell-CHSH inequality.

IV. BELL DISCORD AND MERMIN DISCORD

Each Bell-CHSH inequality is violated by only one PR-box is a consequence of monogamy between the Bell functions,

\[
\mathcal{B}_{\alpha\beta} := |\langle A_0 B_0 \rangle + (-1)^\beta \langle A_0 B_1 \rangle + (-1)^\gamma \langle A_1 B_0 \rangle + (-1)^{\alpha\beta\gamma\epsilon} \langle A_1 B_1 \rangle|.
\]

(15)

The Bell function monogamy is given as follows,

\[
\mathcal{B}_{00} + \mathcal{B}_j \leq 4, \quad \forall j = 01, 10, 11.
\]

(16)

The above monogamy implies that for a single PR-box only one of the Bell functions attains its maximum and the rest of them take zero. The isotropic PR-box,

\[
P = p_P^{\alpha\beta\gamma} + (1 - p) P_N,
\]

(17)

has the special property that only one of the Bell functions is nonzero which is due to the single PR-box, \(P_P^{\alpha\beta\gamma}\), which is irreducible in the decomposition. When \(\alpha\beta\gamma = 000\) in Eq. (17), the box has \(\mathcal{B}_{00} = 4p\) and the rest of the Bell functions are zero.

We now define Bell discord which quantifies irreducible PR-box component in any NS correlation. For this we first construct the following quantities,

\[
\mathcal{G}_1 := |\mathcal{B}_{00} - \mathcal{B}_{01}| - |\mathcal{B}_{10} - \mathcal{B}_{11}|
\]
\[
\mathcal{G}_2 := |\mathcal{B}_{00} - \mathcal{B}_{10} - |\mathcal{B}_{01} - \mathcal{B}_{11}|
\]
\[
\mathcal{G}_3 := |\mathcal{B}_{00} - \mathcal{B}_{11} - |\mathcal{B}_{01} - \mathcal{B}_{10}|
\]

Here \(\mathcal{G}_i\) are connected to each other by LRO. In \(\mathcal{G}_i\), \(\mathcal{B}_{\alpha\beta}\) are subtracted such that \(\mathcal{G}_i\) are zero for all deterministic boxes. Bell discord is defined as follows,

\[
\mathcal{G} := \min_i \mathcal{G}_i.
\]

(18)

and is invariant under LRO, which is a key property required for a nonclassical measure. The measure \(\mathcal{G}\) is symmetric under party’s permutation. The reason for the minimization in Eq. (18) will be explained while deriving the canonical decomposition given in Eq. (23).

The set of \(\mathcal{G} = 0\) boxes forms a subpolytope of the Bell polytope since Bell-local boxes can also have \(\mathcal{G} > 0\). The \(\mathcal{G} = 0\) polytope is nonconvex since certain convex combinations of deterministic boxes can have \(\mathcal{G} > 0\).

We now prove that any NS correlation can be written as the convex combination of a irreducible PR-box and a \(\mathcal{G} = 0\) box. The decomposition given in Eq. (12) can be rewritten as the convex combination of the 8 PR-boxes and a restricted Bell-local box that cannot be written as the convex sum of the PR-boxes and the deterministic boxes,

\[
P = \sum_i g_i P_{PR}^i + \left(1 - \sum_k g_k\right) P_L,
\]

(19)

where \(P_L = \sum_k r_k P_{PR}^k + \sum_i s_i P_D^i\). Note that unequal mixture of two PR-boxes can be written as the convex sum of a single PR-box and a Bell-local box: \(P_P^{\alpha\beta\gamma} = q P_{PR}^{\alpha\beta\gamma} + (p - q) P_L\), where \(p > q\), and \(P_L = \frac{1}{2}(P_{PR}^0 + P_{PR}^1)\) which is a Bell-local box since an uniform mixture of two PR-boxes cannot violate a Bell-CHSH inequality. Therefore the convex mixture of the 8 PR-boxes can be rewritten as the convex mixture of an irreducible PR-box and the 7 Bell local boxes which are uniform mixture of two-PR-boxes,

\[
\sum_k g_k P_{PR}^k = G' P_{PR}^{\alpha\beta\gamma} + \sum_i p_i P_L^i.
\]

(20)

provided that \(G'\) is minimized over all possible decomposition i.e., \(\sum_k g_k P_{PR}^k \neq \sum_i q_k P_L^i\) in order to ensure that it is irreducible PR-box component. This minimization is related to the minimization in Eq. (18), which can be illustrated by the following correlation,

\[
P = 0.4P_{000} + 0.3P_{100} + 0.2P_{110} + 0.1P_{110}.
\]

(21)

If we start to combine the first PR-box and the last PR-box in the above decomposition, the resulting correlation can be
written as the convex sum of a single PR-box and a Bell local box,
\[ P = G' P^0_{PR} + (1 - G') P_L, \]
where \( G' = 0.2 \) and \( P_L = \frac{1}{4} P^0_{PR} + \frac{1}{4} P^{10}_{PR} + \frac{1}{4} P^{01}_{PR} + \frac{1}{4} P^{11}_{PR} \). This nonzero \( G' \) cannot be the irreducible PR-box component as \( G' \) vanishes for other possible decompositions, for instance, if we start combining the first PR-box and the second PR-box, \( G' \) will vanish. For this correlations, \( G_1 = G_2 = 0 \) and \( G_3 = 0.8 \) which explains why the minimization in Eq. (18) is required. Notice that the calculation of \( G_3 \) for the correlation in Eq. (21) illustrates how the subtraction of \( B_{off} \) made in them serves to calculate the single PR-box component. Now substituting Eq. (20) in Eq. (19), we get the canonical decomposition,
\[ P = G' P^b_{PR} + (1 - G') P^g_{PR}, \]
here \( P^g_{PR} = \frac{1}{4} \left( \sum P_i^g L_i + (1 - \sum P_i^g L_i) \right) \). \( P^0_{PR} \) is a \( G = 0 \) correlation follows from the following geometric intuition: Any NS correlations lies between a line joining the two boxes in the NS polytope. Notice that the Bell-local polytope can be divided into two parts: \( G > 0 \) region and \( G = 0 \) polytope which implies that the Bell local box in Eq. (23) lies inside the \( G = 0 \) polytope since the boundary of this region is closer to the origin (white noise).

\( G \) is linear for the canonical decomposition given in Eq. (23) i.e., \( G(P) = G(G(P^b_{PR})+(1-G')P^g_{PR}) \) which implies \( G = 4G' \). The violation of Bell-CHSH inequality is only a sufficient condition for irreducible PR-box component. Suppose \( P^b_{PR} = P^0_{PR} \) in Eq. (23), the box gives \( B_{000} = 4G' + l(1-G') \), where \( l = B_{000} \). We get \( B_{000} > 2 \) if \( G' > \frac{2-l}{4} \), whereas \( G > 0 \) if \( G' > 0 \).

**Mermin boxes.** Bell polytope admits two types of Mermin boxes which can show contextual argument presented in Sec. II. The distinction between the two types of Mermin boxes is achieved by their marginals. They are 32 non-quantum Mermin boxes which have nonmaximally mixed marginals:
\[ P^b_{M} = \frac{1}{2} \left( \delta_{i m} \delta_{j n} + \delta_{m j} \delta_{i n} \right), \]
\[ P^{g}_{M} = \frac{1}{2} \left( \delta_{i m} \delta_{j n} + \delta_{m j} \delta_{i n} \right), \]
and 8 quantum Mermin boxes which have maximally mixed marginals,
\[ P^b_{M}(a_m,b_n|a_i,B_j) = \begin{cases} 0, & i, j \neq 0 \\ 1, & (i \oplus j) \oplus a_i \oplus a_j \\ 0, & \text{otherwise}, \end{cases} \]
\[ P^g_{M}(a_m,b_n|a_i,B_j) = \begin{cases} 0, & i, j \neq 0 \\ 1, & (i \oplus j) \oplus a_i \oplus a_j \\ 0, & \text{otherwise}. \end{cases} \]

All the Mermin boxes lie in the faces of the \( G = 0 \) polytope. A Mermin box is an uniform mixture of two nonlocal boxes which violate the Bell-CHSH inequality maximally: a non-quantum Mermin box is an uniform mixture of two nonlocal deterministic boxes, whereas a quantum Mermin box is an uniform mixture of two PR-boxes. An uniform mixture of two PR-boxes can also give rise to white noise, but a Mermin box is a special kind of Bell local box that retains contextuality while nonlocality is disappeared by the uniform mixture. The following analogy would help us to understand how the Mermin box is contextual despite it is local: A PR-box is an uniform mixture of two nonlocal deterministic boxes, for instance,
\[ P^0_{PR} = \frac{1}{2} \left( \delta_m \delta_n + \delta_m \delta_n \right). \]

In the above decomposition, the uniform mixture of two signaling boxes makes the box to be nonsignaling, however, nonlocality is retained since the box maximally violates the Bell-CHSH inequality. The uniform mixture of two PR-boxes in the following Mermin box,
\[ P^b_{M} = \frac{1}{2} \left( P_{PR} + P^1_{PR} \right), \]
makes the box to be local, however, contextuality of the box is not fully disappeared.

**Mermin discord.** We consider the complete set of Mermin inequalities,
\[ M_{off} := (\alpha \oplus \beta \oplus 1)(-1)^{\alpha\beta\gamma}(A_0B_1) \]
\[ + (\alpha \oplus \beta)(-1)^{\alpha\beta\gamma}(A_0B_0) \]
\[ + (-1)^{\alpha\beta\gamma}(A_1B_1) \leq 2. \]

These Mermin inequalities do not distinguish between contextual correlation and noncontextual correlation, however, magnitude of modulus of the Mermin functions \( M_{off} \):
\[ M_{off} := (\alpha \oplus \beta \oplus 1)(-1)^{\alpha\beta\gamma}(A_0B_1) \]
\[ + (\alpha \oplus \beta)(-1)^{\alpha\beta\gamma}(A_0B_0) \]
\[ + (-1)^{\alpha\beta\gamma}(A_1B_1) \leq 2. \]

serve to construct Mermin discord which detects irreducible Mermin box. For any Mermin box only one of the Mermin functions, \( M_{off} \), takes 2 and the rest of them take zero, whereas for the deterministic boxes and the PR-boxes two Mermin functions take 2 and the rest of them are zero. Similar to Bell discord, we define Mermin discord using \( M_{off} \) as follows:
\[ Q := \min_j Q_j, \]
where, \( Q_j = \min |M_{00} - M_{01}| - |M_{10} - M_{11}| \), and \( Q_2 \) and \( Q_3 \) are obtained by permuting \( M_{off} \) in \( Q_1 \). Here \( 0 \leq Q \leq 2 \).

The measure \( Q \) divides the \( G = 0 \) polytope into \( Q > 0 \) region and \( Q = 0 \) polytope whose vertices are the deterministic boxes. This division of \( G = 0 \) polytope allows us to decompose \( G = 0 \) correlation in Eq. (23) as the convex sum of a \( Q = 2 \) correlation and a \( G = 0 \) correlation:
\[ P^g_{L} = q_M Q_{2} + (1 - q_M) P^g_{L}. \]
where $P_{Q=2}$ is, in general, convex combination of the three Mermin boxes, $P_{Q=2} = uP_{M}^{M} + vP_{M}^{m} + wP_{M}^{m}$, where $P_{M}^{m} = 1/4(\rho_{M}^{M} + \rho_{M}^{m})$ is a quantum Mermin box and, $P_{M}^{M}$ and $P_{M}^{m}$ are the non-quantum Mermin boxes.

**Monogamy between the measures** - Substituting Eq. (33) in Eq. (33), we get,

$$P = G^{'T}_{PR} + Q^{'T}_{PR} + (1 - G^{'T} - Q^{'T})P_{Q=0}^{Q=0},$$

where $Q^{'T} = (1 - G^{'T})q_{M}$. Evaluation of Mermin discord for the decomposition in Eq. (34) gives, $Q(P) = GQ(P_{PR}^{PR}) + QQ(P_{Q=2}) + (1 - G - Q)Q(P_{Q=0}) = 2Q$. Geometrically, any NS correlation lies inside the three dimensional plane formed by a PR-box, a $Q = 2$ box and a $G = Q = 0$ box. The probability constraint $G^{'T} + Q^{'T} \leq 1$ implies the monogamy between the two measures,

$$G + 2Q \leq 4.$$

**V. QUANTUM CORRELATIONS**

Here we study the correlations arising from the quantum states associated with the bipartite Bell-CHSH scenario. The joint state of two spin-1/2 (qubit) particles is given by the density operator $\rho_{AB}$ in the complex vector space $\mathcal{L}(\mathcal{H}_{A}^{2} \otimes \mathcal{H}_{B}^{2})$, which in the Bloch representation can be expressed as follows:

$$\rho_{AB} = \frac{1}{4} \left( I \otimes I + \sum_{i} r_{i} \sigma_{i} \otimes I + \sum_{i} s_{i} I \otimes \sigma_{i} + \sum_{ij} T_{ij} \sigma_{i} \otimes \sigma_{j} \right),$$

where $\sigma_{i}$, $i = 1, 2, 3$, are the Pauli matrices, where $r_{i} = \text{Tr}(\rho_{AB} \sigma_{i} \otimes I)$ and $s_{i} = \text{Tr}(\rho_{AB} I \otimes \sigma_{i})$ are the local Bloch vectors, and $T_{ij} = \text{Tr}(\rho_{AB} \sigma_{i} \otimes \sigma_{j})$ is the correlation tensor. Alice and Bob generate $P(a_{m}, b_{n} | A_{i}, B_{j})$ by making spin projective measurements on their qubits along the directions $\hat{a}_{i}$ and $\hat{b}_{j}$. We show that a quantum-quantum (QQ) state can give rise to (1) a Bell discordant box which has $G > 0$ and $Q = 0$, (2) a Mermin discordant box which has $G = 0$ and $Q > 0$, and (3) a Bell-Mermin discordant box which has $G > 0$ and $Q > 0$, for three different incompatible measurements.

**A. Schmidt states**

We consider the correlations arising from the Schmidt states (pure entangled states $|14\rangle$):

$$\rho_{S} = \frac{1}{4} \left( I \otimes I + c(\sigma_{x} \otimes I + I \otimes \sigma_{x}) + s(\sigma_{z} \otimes \sigma_{y} - \sigma_{y} \otimes \sigma_{z}) + t(\sigma_{x} \otimes \sigma_{y} + \sigma_{y} \otimes \sigma_{x}) \right),$$

where $c = \cos 2\theta$, $s = \sin 2\theta$ and $0 < \theta \leq \frac{\pi}{4}$. The Schmidt states can give rise to (i) a maximally mixed marginals box when measurements performed in the $xy$-plane or (ii) a non-maximally mixed marginals box when measurements performed in the $xz$-plane.

**1. Bell-Schmidt box**

(i) The Schmidt states give to the noisy PR-box:

$$P = \frac{s}{\sqrt{2}}P_{PR} + \left(1 - \frac{s}{\sqrt{2}}\right)P_{N},$$

for the measurement settings: $\hat{d}_{0} = \hat{x}$, $\hat{d}_{1} = \hat{y}$, $\hat{b}_{0} = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y})$ and $\hat{b}_{1} = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y})$. The correlations have $B_{\theta_{0}} = 2\sqrt{s}$ and the rest of the Bell functions are zero, which gives $G = 2\sqrt{s}$ and $Q = 0$. The box violates the Bell-CHSH inequality if $s > \frac{1}{\sqrt{2}}$ and gives rise to nonzero Bell discord if $s > 0$. When $0 < s \leq \frac{1}{\sqrt{2}}$, the box is Bell local yet it is Bell discordant due to nonzero PR-box component.

(ii) Popescu and Rohrlich showed that all the Schmidt states violates the Bell-CHSH inequality $|15\rangle$. For instance, the settings: $\hat{d}_{0} = \hat{x}$, $\hat{d}_{1} = \hat{x}$, $\hat{b}_{0} = \cos\hat{t}_{x} + \sin\hat{t}_{x}$ and $\hat{b}_{1} = \cos\hat{t}_{x} - \sin\hat{t}_{x}$, where $\cos t = \frac{1}{\sqrt{1 + t^2}}$, gives rise to $B_{\theta_{0}} = 2\sqrt{1 + s^2}$, $B_{\theta_{1}} = \frac{2s}{\sqrt{1 + t^2}}$, and $B_{\theta_{0}} = B_{\theta_{1}} = 0$, which implies $G = \frac{4\sqrt{s}}{1 + t^2}$ and $Q = 0$. Since $B_{\theta_{0}} > 2$ if $s > 0$, the correlation is Bell nonlocal if the state is entangled. Since the box has nonmaximally mixed marginals, it has less irreducible PR-box component than the correlations in Eq. (40).

**2. Mermin-Schmidt box**

The complete set of EPR-steering inequalities,

$$\cal{M}_{0}^{dy} \leq \sqrt{2},$$

put upper bound on the correlations under the constraint that measurements on Alice’s or Bob’s side are anti-commuting quantum observables.

(i) For the settings, $\hat{d}_{0} = \hat{x}$, $\hat{d}_{1} = -\hat{y}$, $\hat{b}_{0} = \hat{y}$ and $\hat{b}_{1} = \hat{x}$, the Schmidt states give rise to the noisy Mermin-box:

$$P = \frac{s}{2} \left( P_{PR}^{00} + P_{PR}^{11} \right) + (1 - s)P_{N}. \tag{40}$$

This box has $\mathcal{M}_{00} = 2s$, and, $\mathcal{M}_{01} = \mathcal{M}_{10} = \mathcal{M}_{11} = 0$, which gives $Q = 2s$ and $G = 0$. This Bell local box violates the EPR-steering inequality if $s > \frac{1}{\sqrt{2}}$, and has Mermin discord if $s > 0$. When $0 < s \leq \frac{1}{\sqrt{2}}$, the box does not violate the EPR-steering inequality yet it has Mermin discord because of nonzero Mermin box component.

(ii) All the Schmidt states violate the EPR-steering inequality for the settings, $\hat{d}_{0} = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y})$, $\hat{d}_{1} = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y})$, $\hat{b}_{0} = \cos\hat{t}_{x} + \sin\hat{t}_{x}$, and $\hat{b}_{1} = \cos\hat{t}_{x} - \sin\hat{t}_{x}$, where $\cos t = \frac{1}{\sqrt{1 + t^2}}$.

For this settings, the Schmidt states give, $\mathcal{M}_{00} = \frac{\sqrt{2}s}{\sqrt{1 + t^2}}$, $\mathcal{M}_{01} = \mathcal{M}_{10} = 0$ and $\mathcal{M}_{11} = \sqrt{2}\sqrt{1 + s^2}$, which implies $Q = \frac{2\sqrt{s}}{\sqrt{1 + t^2}}$ and $G = 0$. Since the correlations has nonmaximally mixed marginals, it has less irreducible Mermin box component than the correlations in Eq. (40).
3. Bell-Mermin-Schmidt box

(i) The following decomposition for correlations:

\[
P = (1 - |q| - |r|)P_N + \frac{|q|}{2} \left( p_{PR}^{000} + p_{PR}^{111} \right) + |r| \left( \frac{1}{\sqrt{2}} p_{PR}^{000} + \left( 1 - \frac{1}{\sqrt{2}} \right) P_N \right),
\]

(41)
is achieved when settings is chosen as follows: \( a_0 = s\hat{x} + c\hat{y}, \)
\( a_1 = c\hat{x} - s\hat{y}, \)
\( b_0 = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y}) \) and \( b_1 = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y}), \) where,
\[ q = \sqrt{\frac{|d - c| + s}{2}} \] and \( r = s(s - c). \) The box gives,
\[ G = 2\sqrt{2}s|s - c| > 0 \quad \text{except when} \quad \theta \neq 0, \frac{\pi}{4}, \]
\[ Q = s\sqrt{2}|c + s| - |c - s| > 0 \quad \text{except when} \quad \theta \neq 0, \frac{\pi}{4}, \]
\[ = 2\sqrt{2}s^2 \quad \text{when} \quad c > s \]
\[ = 2\sqrt{2}cs \quad \text{when} \quad s > c. \]

(ii) We define the settings: \( a_0 = c\hat{x} + s\hat{z}, \)
\( a_1 = s\hat{x} - c\hat{z}, \)
\( b_0 = \frac{1}{\sqrt{2}}(\hat{x} + \hat{z}) \) and \( b_1 = \frac{1}{\sqrt{2}}(-\hat{x} + \hat{z}), \) which gives,
\[ G = 2\sqrt{2}s|s - c| > 0 \quad \text{except when} \quad \theta \neq 0, \frac{\pi}{4}, \]
\[ Q = s\sqrt{2}|c + s| - |c - s| > 0 \quad \text{except when} \quad \theta \neq 0, \frac{\pi}{4}, \]
\[ = 2\sqrt{2}s^2 \quad \text{when} \quad c > s \]
\[ = 2\sqrt{2}cs \quad \text{when} \quad s > c. \]

We see that \( G \) and \( Q \) for the latter settings (ii) is less than that for the former settings (i) since the latter correlations have nonmaximally mixed marginals.

B. Werner states

Consider the correlations due to the Werner states,
\[ \rho_W = p|\psi^+\rangle\langle\psi^+| + (1 - p)\frac{1}{4}. \]

(42)
The Werner states are entangled if \( p > \frac{1}{2} \) and have nonzero quantum discord if \( p > 0.17 \). We show that the Werner states can have Bell discord or Mermin discord if \( p > 0. \) The Werner states can only give rise to maximally mixed marginals correlations.

1. Bell-Werner box

The correlations has the following decomposition,
\[ P = p \left( \frac{1}{\sqrt{2}} p_{PR}^{000} + \left( 1 - \frac{1}{\sqrt{2}} \right) P_N \right) + (1 - p)P_N. \]

(43)

for the settings that corresponds to the decomposition in Eq. (38), which gives \( G = 2\sqrt{Z}p. \) The correlations violates the Bell-CHSH inequality if \( p > \frac{1}{\sqrt{2}}, \) however, it has nonzero Bell discord if \( p > 0. \)

2. Mermin-Werner box

The Werner states give rise to the nosisy Mermin box,
\[ P = (1 - p)P_N + \frac{q}{2} (p_{PR}^{000} + p_{PR}^{111}) + |r| p_{PR}^{000}, \]

(44)
which gives \( Q = 2p, \) for the settings corresponding to the decomposition in Eq. (10). The correlations does not violate a Bell-CHSH inequality but violates the EPR-steering inequality if \( p > \frac{1}{\sqrt{2}}, \) and has nonzero Mermin discord if \( p > 0. \)

3. Bell-Mermin-Werner box

The Werner states admit the following decomposition:
\[ P = (1 - q - r)P_N + \frac{q}{2} (p_{PR}^{000} + p_{PR}^{111}) + |r| p_{PR}^{000}, \]

(45)
when the settings are chosen as follows: \( a_0 = \sqrt{p}\hat{x} + \sqrt{1 - p}\hat{y}, \)
\( a_1 = \sqrt{1 - p}\hat{x} - \sqrt{p}\hat{y}, \)
\( b_0 = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y}) \) and \( b_1 = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y}), \) where, \( q = p\sqrt{2(1 - p)} \) and \( r = \frac{1}{\sqrt{2}}p(\sqrt{p} - \sqrt{1 - p}). \) The box gives
\[ G = 2\sqrt{2}p|\sqrt{p} - \sqrt{1 - p}| > 0 \quad \text{except when} \quad p \neq 0, \frac{1}{2}, \]
\[ Q = 2p\sqrt{2(1 - p)} > 0 \quad \text{except when} \quad p \neq 0, 1. \]

C. Mixture of maximally entangled state with colored noise

We consider correlations arising from the mixture of the Bell state and the classically correlated state,
\[ p = p|\psi^+\rangle\langle\psi^+| + (1 - p)\rho_{CC}, \]

(46)
where \( \rho_{CC} = \frac{1}{2}(|00\rangle\langle00| + |11\rangle\langle11|). \) When measurements performed on the \( xy \)-plane, the states have the same behaviour as the Werner states. Measurements in the \( xz \)-plane plane distinguishes these states from the Werner states. For instance, consider the Bell discordant correlations:

(i) The settings which gives the noisy PR-box in Eq. (38), gives \( B_0 = 2\sqrt{2}p > 2 \) if \( p > \frac{1}{\sqrt{2}}, \) \( B_{01} = B_{10} = B_{11} = 0 \) and \( G = 2\sqrt{2}p > 0 \) if \( p > 0. \)

(ii) The measurement settings, \( a_0 = \hat{z}, a_1 = \hat{x}, b_0 = \text{cos} t\hat{z} + \text{sin} t\hat{x} \) and \( b_1 = \text{cos} t\hat{z} - \text{sin} t\hat{x}, \) where \( \text{cos} t = \frac{1}{\sqrt{1 + p^2}}, \) gives,
\[ B_{00} = 2\sqrt{1 + p^2} > 2 \] if \( p > 0, \)
\[ B_{11} = \frac{2(1 - p)^2}{\sqrt{1 + p^2}}, \]
\[ B_{01} = B_{10} = 0, \]
and \( G = \frac{4p^2}{\sqrt{1 + p^2}}. \)
Thus we see that when we perform incompatible measurements in the $xz$-plane, the states have different nonclassical behaviour than the Werner states.

### D. Classical-quantum and quantum-classical states

Here we show that all classical-quantum (CQ) states and quantum-classical (QC) states have $G = Q = 0$ for all measurements settings. The CQ states can be written as,

$$
\rho = \sum_{i=0}^{1} p_i |i\rangle\langle i| \otimes \chi_i,
$$

whereas, the QC states can be written as,

$$
\rho = \sum_{j=0}^{1} p_j |j\rangle\langle j|.
$$

where $|i\rangle$ and $|j\rangle$ are the orthonormal sets on Alice’s and Bob’s side and $\chi_i$ and $\phi_j$ are the quantum states.

The analysis in the previous sections shows that the optimal settings have the following property: for the Bell discord one has, $\hat{a}_0 \cdot \hat{r} = 0, \hat{b}_0 \cdot \hat{b}_1 = 0$ and $\hat{a}_1 \cdot \hat{b}_j = \pm \frac{1}{\sqrt{2}}$, whereas for the Mermin discord one has: $\hat{a}_0 \cdot \hat{a}_1 = 0, \hat{b}_0 \cdot \hat{b}_1 = 0$ and $\hat{a}_i \cdot \hat{b}_j$. Despite the CQ and QC states are not the product states, their joint expectations values can be written in the product state like form. $\langle AB \rangle = f(\hat{a})f(\hat{b})$, which resembles that of the product states. This factorization of the expectation values for the CQ states and QC states implies that they cannot have non-zero Bell discord or non-zero Mermin discord.

**Proof**. In the Bloch sphere representation, the CQ state in Eq. (47) can be written as:

$$
\rho_{AB} = \frac{p_0}{4} \mathbb{1} + \hat{x}' \cdot \sigma_x \mathbb{1} + \hat{y}' \cdot \sigma_y \mathbb{1} + \hat{z}' \cdot \sigma_z \mathbb{1} + \frac{p_1}{4} \mathbb{1} - \hat{x}' \cdot \sigma_x \mathbb{1} - \hat{y}' \cdot \sigma_y \mathbb{1} - \hat{z}' \cdot \sigma_z \mathbb{1}.
$$

$$
B_{\rho_{AB}} = \frac{1}{\sqrt{2}} \sqrt{((\sigma_x \otimes \sigma_x) + (-1)^{\hat{y}} \sigma_x \otimes (\sigma_x - \sigma_y) + (-1)^{\hat{y}} \sigma_y \otimes (\sigma_x + \sigma_y) + (-1)^{\hat{x}} \sigma_y \otimes (\sigma_x - \sigma_y))}
$$

$$
= \sqrt{2} \sqrt{((\alpha \otimes \beta \otimes 1)(-1)^{\hat{y}} \sigma_x \otimes \sigma_x) + (-1)^{\hat{y}} \sigma_y \otimes (\sigma_x + \sigma_y) + (-1)^{\hat{x}} \sigma_y \otimes (\sigma_x - \sigma_y))}
$$

$$
= \sqrt{2} M_{\rho_{AB}},
$$

due to the linearity of quantum theory, $\langle A + B \rangle = \langle A \rangle + \langle B \rangle$. The relationship between the Bell functions and the Mermin function given in Eq. (53) implies that for any maximally entangled state $\rho_{me}$, maximal Bell discord and Mermin discord are related as follows: $G_{\text{max}}(\rho_{me}) = \sqrt{2}Q(\rho_{me})$, which implies, $G_{\text{max}}(\rho) = 2\sqrt{2}$ since $Q_{\text{max}} = 2$.

If we constrain the Bell polytope by maximally mixed marginals, we will get a polytope whose vertices are the colored

$$
\langle A, B \rangle = (\hat{a}_i \cdot \hat{r}) \left( \hat{b}_j \cdot (p_0 \hat{s}_0 - p_1 \hat{s}_1) \right),
$$

whose form is similar to that of a product state, $\rho = \frac{1}{2}[(\mathbb{1} + \hat{r} \cdot \sigma_0 \mathbb{1} + \hat{r} \cdot \sigma_0 \mathbb{1})$, which in turn, implies $G = 0$ and $Q = 0$.

**E. Tsirelson bound**

Consider a subpolytope of NS polytope whose vertices are the 8 noisy PR-boxes that corresponds to Tsirelson bound,

$$
P_{\text{PR}}^{\gamma_{\text{PR}}} = \frac{1}{\sqrt{2}} P_{\text{PR}}^{\gamma_{\text{PR}}} + (1 - \frac{1}{\sqrt{2}}) P_{\text{N}},
$$

and 8 Mermin-boxes with maximally mixed marginals. This polytope can be simulated by quantum theory. For instance, the convex mixture of the 8 maximally entangled states,

$$
\rho = p_1 |\psi^+\rangle\langle \psi^+| + q_1 |\phi^+\rangle\langle \phi^+|,
$$

where $|\psi^+\rangle = \frac{1}{\sqrt{2}}(00 + (-1)^{\hat{y}} 11)$ and $|\phi^+\rangle = \frac{1}{\sqrt{2}}(01 + (-1)^{\hat{y}} 10)$, can simulate the entire region for the three different measurement settings. In this polytope, Mermin discord limits Bell discord to Tsirelson bound. Consider following measurement settings: $a_0 = \hat{x}, a_1 = \hat{y}, b_0 = \frac{1}{\sqrt{2}}(\hat{x} + \hat{y})$, and $b_1 = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y})$, which maximizes $G$. For this settings, the Bell functions reduce to the Mermin functions as follows:

$$
G_{\text{max}}(\rho) = \sqrt{2}Q(\rho_{me}),
$$

boxes,

$$
P_{\text{CC}}^{\gamma_{\text{CC}}} (a_m, b_n | A_i, B_j) = \begin{cases} 1/2, & m \oplus n = ai + bj + \gamma \\ 0, & \text{otherwise} \end{cases}
$$

If we constrain the colored box polytope by Mermin discord, we will get Mermin box polytope whose vertices are the 8 Mermin boxes which have maximally mixed marginals. This Mermin box polytope is purely a quantum region as it can be simulated by the quantum theory. Therefore the constraints
maximal local randomness and Mermin discord in GNST would single out quantum theory.

VI. CONCLUSIONS

We found that full NS polytope can be divided into four parts: (i) $G > 0$ & $Q = 0$ region (ii) $G = 0$ & $Q > 0$ region (iii) $G > 0$ & $Q > 0$ region and (iv) $G = Q = 0$ polytope. This division allows us to characterize any NS correlation as a point lies inside the three dimensional plane formed by a PR-box, a $Q = 2$ box and a $G = Q = 0$ box. We showed that the nonclassicality of Bell-local boxes is due to the irreducible PR-box component or the irreducible Mermin-box component.

Our analysis shows that in GNST, all pure and mixed quantum states are treated on an equal footing that it is the convex mixture of a PR-box, a Mermin box and a $G = Q = 0$ box. Quantum correlations which have the overlap with the three nonclassical regions of the NS polytope can be generated by the QQ states for three different choices of measurement settings, whereas the CQ states and QC states are mapped into the $G = Q = 0$ polytope.

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