

Interference in quantum correlations

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We show that the expectation values of operators of multiparticle systems consist of two contributions: (1) one that solely involves probabilities and (2) one arising from interference. We demonstrate that a nonvanishing interference contribution is necessary to either surpass classical bounds, such as the Clauser-Horne-Shimony-Holt border, or create contradictions to classical predictions, as in the Greenberger-Horne-Zeilinger scenario.

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I. INTRODUCTION

Quantum interference [1] and entanglement [2,3] are two of the striking properties that make quantum mechanics a nonclassical theory. This distinction between classical and quantum physics is most evident, among others, in Bell's theorem [4] and its variations, for example, the Clauser-Horne-Shimony-Holt (CHSH) inequality [5] or the Hardy scenario [6,7] for bipartite systems, or the Greenberger-Horne-Zeilinger (GHZ) [8,9] arrangement for multiparticle systems.

A recent article [10] has demonstrated that all Hardy conditions [6,7] and the violation of their classical consequences are only fulfilled when several probability amplitudes interfere destructively. Thus, different predictions based on a quantum and a classical description are again rooted in quantum interference.

In this article, we generalize the principle of quantum interference arising in the Hardy scenario to expectation values of arbitrary multipartite systems. Our key tool is a decomposition of the expectation value into two contributions, one arising from probabilities and one containing the interference terms. We emphasize that such a decomposition depends on the choice of the measurement basis. We illustrate our formalism by applying it to two special examples, the CHSH inequality and the GHZ scenario. The flowchart in Fig. 1 summarizes those key ideas.

The CHSH problem considers the sum of four expectation values involving four measurements on this bipartite system. As we will show in this article, it is the effect of interfering probability amplitudes that leads to the violation of the CHSH inequality.

In the GHZ scenario, we consider four expectation values of three measurements. We demonstrate that when we choose the measurement basis appropriately, the expectation values leading to a contradiction arise solely from interference, since the probabilistic contribution vanishes.

Our article is structured as follows: In Sec. II, we point out that the choice of the measurement basis dictates the structure of the expectation value of a product of operators. In particular, we show that a measurement basis that is not the eigenbasis of the measurement operator leads to interfering probability amplitudes. Moreover, in Sec. III, we investigate the conditions under which the interference vanishes. Here, the state and the measurements play a crucial role.

While we keep the discussion in the first three sections general by considering Hermitian measurement operators acting on arbitrary multipartite entangled systems of n subspaces, we adapt in Secs. IV and V the principle of interference to two specific examples. In Sec. IV, we identify interference of probability amplitudes as the crucial ingredient that allows the CHSH inequality to exceed its classical bounds. Furthermore, a bipartite system allows for a schematic illustration of interfering probability amplitudes as connections between the corners in a three-dimensional cube. In Sec. V, we adapt the same principle to a special measurement arrangement describing the GHZ scenario and show that the contradiction between classical and quantum theory requires interference.

In Sec. VI, we finally conclude with a short summary. Moreover, we present a brief outlook.

In addition, we provide three appendices. In Appendix A, we derive explicit expressions for the matrix elements connecting the different measurement bases and the probabilistic as well as the interference contribution entering the CHSH expectation value for a specific measurement arrangement. Furthermore, in Appendix B, we present an estimation of the bounds of the probabilistic contribution of the CHSH expectation value without the need for a specific measurement arrangement. Finally, in Appendix C, we derive explicit expressions for the example of measurements maximally violating the CHSH inequality for pure states. In particular, we derive the angles between the measurement directions on

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FIG. 1. Flowchart allowing us to identify the role of interference in multipartite quantum systems.

both subsystems, as well as the expectation value of a joint measurement.

II. n -PARTICLE INTERFERENCE

In order to bring out the fundamental role of interference in quantum mechanics, we consider a system of n subsystems and perform measurements on each of them. In particular, we analyze the expectation values of two different sets of n Hermitian operators. We will show that by expressing the measurement operator in a basis that is not the eigenbasis, the probability to observe a certain measurement outcome results from the interference of several probability amplitudes.

We first calculate these expectation values by representing the operators in their respective eigenbasis. In the next step, we expand the second set of operators in the eigenbasis of the first set. The corresponding probability amplitude is then given by a sum of the product of matrix elements connecting the two bases and the expansion of the state into the eigenbasis of the first set. This approach allows us to separate the terms corresponding to probabilities and interference.

A. Operator product expressed by its eigenbasis

The key feature of quantum mechanics, that is, interference, comes to light when we compare the expectation values

$$\mathcal{O}_n \equiv \langle \hat{A} \otimes \hat{B} \otimes \cdots \otimes \hat{N} \rangle \quad (1)$$

and

$$\mathcal{O}'_n \equiv \langle \hat{A}' \otimes \hat{B}' \otimes \cdots \otimes \hat{N}' \rangle \quad (2)$$

of two sets of n operators $\hat{A}, \hat{B}, \dots, \hat{N}$ and $\hat{A}', \hat{B}', \dots, \hat{N}'$. Here, each operator acts on a single subsystem; that is, $\hat{A}$ and $\hat{A}'$ operate on the subsystem assigned to Alice, $\hat{B}$ and $\hat{B}'$ on the subsystem assigned to Bob, and so on.

In order to evaluate $\mathcal{O}_n$ and $\mathcal{O}'_n$, we use the spectral decomposition

$$\hat{U} \equiv \sum_u u |u\rangle \langle u| \quad (3)$$

and

$$\hat{U}' \equiv \sum_{u'} u' |u'\rangle \langle u'| \quad (4)$$

of every operator $\hat{U} \in \{\hat{A}, \hat{B}, \dots, \hat{N}\}$ and $\hat{U}' \in \{\hat{A}', \hat{B}', \dots, \hat{N}'\}$, given by their eigenvalues u and u' and eigenstates $|u\rangle$ and $|u'\rangle$, respectively.

Thus, the expectation values $\mathcal{O}_n$ and $\mathcal{O}'_n$ read

$$\mathcal{O}_n = \sum_{a,b,\dots,n} ab \cdots n |\langle a, b, \dots, n | \Psi \rangle|^2 \quad (5)$$

and

$$\mathcal{O}'_n = \sum_{a',b',\dots,n'} a'b' \cdots n' |\langle a', b', \dots, n' | \Psi \rangle|^2, \quad (6)$$

where we have assumed a pure but arbitrary entangled state $|\Psi\rangle$. Hence, each combination of joint measurement outcomes is weighted by the probability of the respective outcome.

B. Operator product expressed not in the eigenbasis

In order to relate the expectation values $\mathcal{O}_n$ and $\mathcal{O}'_n$ to each other, we express the probability amplitudes $\langle a, b, \dots, n | \Psi \rangle$ and $\langle a', b', \dots, n' | \Psi \rangle$ that enter into the expectation values in a common basis. Indeed, we now expand the operators $\hat{A}', \hat{B}', \dots, \hat{N}'$ in the eigenbasis of the operators $\hat{A}, \hat{B}, \dots, \hat{N}$, giving rise to interference.

For this purpose, we insert the completeness relation

$$\sum_{a,b,\dots,n} |a\rangle \langle a| \otimes |b\rangle \langle b| \otimes \cdots \otimes |n\rangle \langle n| = \hat{1} \quad (7)$$

into the probability amplitude

$$\langle a', b', \dots, n' | \Psi \rangle = \sum_{a,b,\dots,n} \langle a' | a \rangle \langle b' | b \rangle \cdots \langle n' | n \rangle \langle a, b, \dots, n | \Psi \rangle, \quad (8)$$

where we have made use of the fact that the scalar products separate into their respective subsystems.

It is useful to introduce the matrix elements

$$\mathbf{A}_{a'a} \equiv \langle a' | a \rangle, \quad \mathbf{B}_{b'b} \equiv \langle b' | b \rangle, \dots, \quad \mathbf{N}_{n'n} \equiv \langle n' | n \rangle, \quad (9)$$

which are a measure of the overlap of the two eigenbases, as well as the probability amplitudes

$$\Psi_{ab \cdots n} \equiv \langle a, b, \dots, n | \Psi \rangle \quad (10)$$

to find the state

$$|\Psi\rangle = \sum_{a,b,\dots,n} \Psi_{ab \cdots n} |a, b, \dots, n\rangle, \quad (11)$$

in the $|a, b, \dots, n\rangle$ eigenstate.

With this notation, the probability amplitude of the joint measurement of the second set of operators in the measurement basis defined by the eigenbasis of the first set of operations, Eq. (8), reads

$$\langle a', \dots, n' | \Psi \rangle = \sum_{a,\dots,n} \mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{ab \cdots n}. \quad (12)$$

We note that due to the change of the measurement basis, the probability amplitude is now a sum over all eigenstates of the basis of $\hat{A}, \hat{B}, \dots, \hat{N}$, which we have used to also expand the operators $\hat{A}', \hat{B}', \dots, \hat{N}'$.

C. Identification of interference

According to the Born rule, the probability

$$\text{pr}_{A',B',\dots,N'}(a', b', \dots, n') = |\langle a', b', \dots, n' | \Psi \rangle|^2 \quad (13)$$

to simultaneously obtain the measurement outcomes $a', b', \dots, n'$ in terms of the new measurement basis $|a, b, \dots, n\rangle$ reads

$$\text{pr}_{A',B',\dots,N'}(a', b', \dots, n') = \left| \sum_{a,b,\dots,n} \mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{ab\dots n} \right|^2. \quad (14)$$

In the language of Feynman [1], each product of matrix elements and a probability amplitude in the sum defines a path. Hence, the summation corresponds to a sum of interfering paths.

In order to bring out most clearly the interference contained in this expression, we decompose the summations in Eq. (14) into the two contributions

$$\text{pr}_{A',B',\dots,N'}(a', b', \dots, n') = P_{a',b',\dots,n'} + I_{a',b',\dots,n'}. \quad (15)$$

While the term

$$P_{a',b',\dots,n'} \equiv \sum_{a,b,\dots,n} \text{pr}_{A'|A}(a'|a) \text{pr}_{B'|B}(b'|b) \cdots \times \text{pr}_{N'|N}(n'|n) \text{pr}_{a,b,\dots,n}(a, b, \dots, n) \quad (16)$$

solely consists of probabilities, that is, conditional probabilities $\text{pr}_{A'|A}(a'|a) \equiv |\mathbf{A}_{a'a}|^2$, $\text{pr}_{B'|B}(b'|b) \equiv |\mathbf{B}_{b'b}|^2$, and $\text{pr}_{N'|N}(n'|n) \equiv |\mathbf{N}_{n'n}|^2$, as well as joint probabilities $\text{pr}_{a,b,\dots,n}(a, b, \dots, n) \equiv |\Psi_{ab\dots n}|^2$, the second contribution

$$I_{a',b',\dots,n'} \equiv \sum_{(a,b,\dots,n) \neq (\tilde{a}, \tilde{b}, \dots, \tilde{n})} \mathbf{A}_{a'a} \mathbf{A}_{\tilde{a}'\tilde{a}}^* \mathbf{B}_{b'b} \mathbf{B}_{\tilde{b}'\tilde{b}}^* \cdots \mathbf{N}_{n'n} \mathbf{N}_{\tilde{n}'\tilde{n}}^* \times \Psi_{ab\dots n} \Psi_{\tilde{a}\tilde{b}\dots\tilde{n}}^* \quad (17)$$

contains all cross terms that arise from interference. Here, the notation $(a, b, \dots, n) \neq (\tilde{a}, \tilde{b}, \dots, \tilde{n})$ in Eq. (17) indicates that at least two indices are different, while we still sum up over all indices.

Hence, the choice of the measurement basis dictates the decomposition of the joint probability $\text{pr}_{A',B',\dots,N'}(a', b', \dots, n')$ into the probability term P and the interference term I .

We conclude by returning to the calculation of the expectation value $\mathcal{O}'_n$ and substitute the decomposition Eq. (15) into Eq. (6), which leads us to the representation

$$\mathcal{O}'_n = \mathcal{O}'_P + \mathcal{O}'_I, \quad (18)$$

consisting of the contribution

$$\mathcal{O}'_P \equiv \sum_{a',b',\dots,n'} a', b', \dots, n' P_{a',b',\dots,n'} \quad (19)$$

arising from the probability term and the contribution

$$\mathcal{O}'_I \equiv \sum_{a',b',\dots,n'} a', b', \dots, n' I_{a',b',\dots,n'} \quad (20)$$

reflecting the interference. Here, we sum over all eigenvalues $a', b', \dots, n'$.

III. MEASUREMENT AND STATE DETERMINATION OR ABSENCE OF INTERFERENCE

In order to get a better understanding of the role of interference, we identify conditions for a vanishing interference contribution. Moreover, we connect several types of measurements and states with interference.

A. Vanishing interference contribution

We show that the interference contribution vanishes when the two sets of operators commute, or when the state is separable and an eigenstate of the measurement operators.

To eliminate the interference in the expectation value $\mathcal{O}'_n$, the interference arising in the probability amplitudes needs to vanish for every single measurement outcome. This scenario takes place when only one of the terms of the sum

$$|\langle a', b', \dots, n' | \Psi \rangle|^2 = \left| \sum_{a,b,\dots,n} \mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{ab\dots n} \right|^2 \quad (21)$$

determining the probability survives, leading us to the expression

$$|\langle a', b', \dots, n' | \Psi \rangle|^2 = |\mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{\alpha\beta\dots\nu}|^2, \quad (22)$$

which requires the condition

$$\mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{ab\dots n} = \delta_{a\alpha} \delta_{b\beta} \cdots \delta_{n\nu} \mathbf{A}_{a'a} \mathbf{B}_{b'b} \cdots \mathbf{N}_{n'n} \Psi_{\alpha\beta\dots\nu}. \quad (23)$$

There are two possibilities leading to the collapse of the sum: (1) the products of the matrix elements reduce to one single term, that is,

$$\mathbf{A}_{a'a} = \delta_{a\alpha} \mathbf{A}_{a'a}, \quad \mathbf{B}_{b'b} = \delta_{b\beta} \mathbf{B}_{b'b}, \dots, \quad \mathbf{N}_{n'n} = \delta_{n\nu} \mathbf{N}_{n'n}, \quad (24)$$

or (2) there exists only a single nonvanishing probability amplitude

$$\Psi_{ab\dots n} = \delta_{a\alpha} \delta_{b\beta} \cdots \delta_{n\nu} \Psi_{\alpha\beta\dots\nu}. \quad (25)$$

These two possibilities are reflected in Eq. (23) by the fact that the product of the Kronecker delta arises either from the product of the matrix elements or from the probability amplitudes.

1. Commuting measurements

We start our discussion by addressing case (1) and note the normalization condition

$$\sum_a |\mathbf{A}_{a'a}|^2 = \sum_a \langle a'|a \rangle \langle a|a' \rangle = \langle a'|\hat{1}|a' \rangle = 1, \quad (26)$$

which follows from the definition, Eq. (9), of the matrix elements together with the completeness relation of the eigenstates $|a\rangle$. Obviously, the same condition also holds for all other matrix elements $|\mathbf{B}_{b'b}|^2, \dots, |\mathbf{N}_{n'n}|^2$.

When we substitute the matrix element, Eq. (24), into the normalization condition, we arrive at the identity

$$|\mathbf{A}_{a'a}|^2 = 1, \quad |\mathbf{B}_{b'b}|^2 = 1, \dots, \quad |\mathbf{N}_{n'n}|^2 = 1, \quad (27)$$

indicating that the matrix elements

$$\mathbf{A}_{a'a} = \langle a'|a \rangle = e^{i\varphi_{a'a}} \quad (28)$$

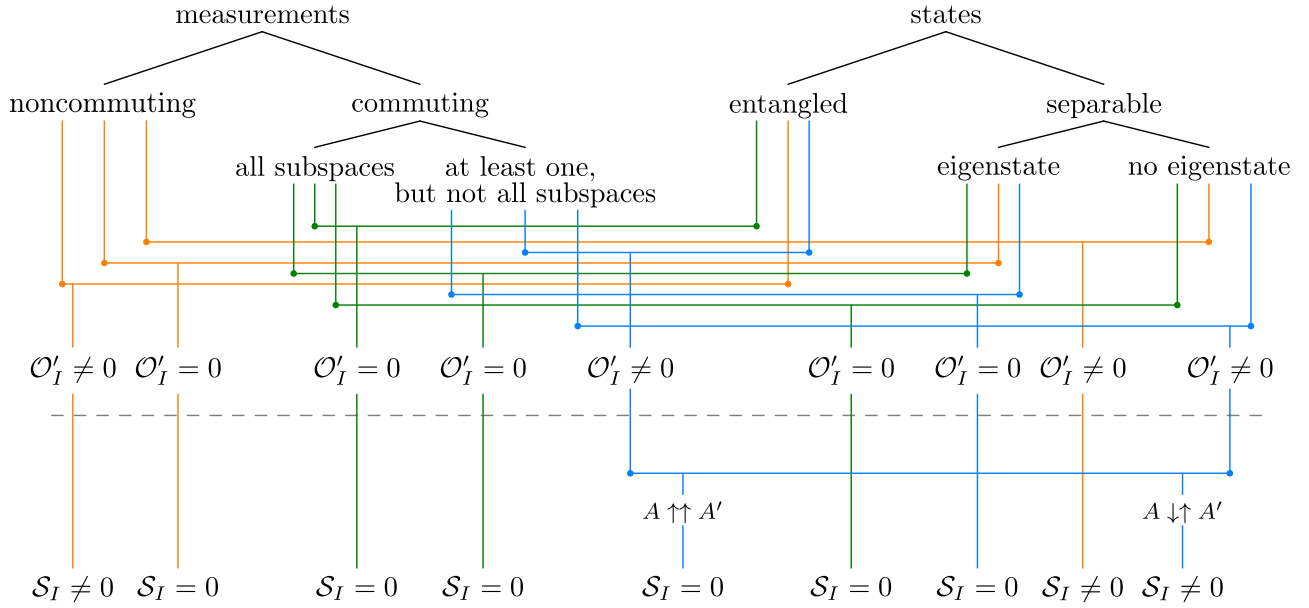


FIG. 2. Transit map connecting measurements and states with the interference contribution $\mathcal{O}'_I$. Lines of different colors always connect measurements and states, and terminate in a prediction of interference, $\mathcal{O}'_I \neq 0$, or no interference, $\mathcal{O}'_I = 0$. The three brown, green, and blue lines start from three different classes of measurements, that is, noncommuting measurements, measurements that commute in all subspaces, and measurements that commute in at least one but not all subspaces, respectively. The rows below the dashed line address the special case of a bipartite system giving rise to the CHSH inequality and discuss the interference term S_I of the Bell sum. Here, we distinguish the cases of the measurement directions A and A' being either parallel or antiparallel.

are phase factors, and the two states $|a'\rangle$ and $|\alpha\rangle$ only differ in a phase $\varphi_{a'\alpha}$, that is,

$$|\alpha\rangle = e^{i\varphi_{a'\alpha}} |a'\rangle. \quad (29)$$

The collapse of the sums due to the matrix elements rather than the probability amplitudes is intimately connected to the commutativity of the measurements, that is, the commutator

$$[\hat{A}, \hat{A}'] = \sum_{a,a'} aa' (\mathbf{A}_{a'a}^* |a\rangle \langle a'| - \mathbf{A}_{a'a} |a'\rangle \langle a|) \quad (30)$$

of the operators $\hat{A}$ and $\hat{A}'$. Here, we have recalled the definition, Eq. (9), of the matrix elements.

With the help of the Kronecker deltas in Eq. (24), the double sum reduces to a single sum, and we find the relation

$$[\hat{A}, \hat{A}'] = \sum_{a'} \alpha a' (\mathbf{A}_{a'a}^* |\alpha\rangle \langle a'| - \mathbf{A}_{a'a} |a'\rangle \langle \alpha|), \quad (31)$$

which with the explicit form, Eq. (28), of the matrix element and the connection, Eq. (29), between the two states $|\alpha\rangle$ and $|a'\rangle$ yields

$$[\hat{A}, \hat{A}'] = \sum_{a'} \alpha a' (|a'\rangle \langle a'| - |a'\rangle \langle a'|) = 0. \quad (32)$$

We recall from Eq. (24) that in order for the interference to vanish, all operators $\hat{B}$ and $\hat{B}', \dots, \hat{N}$ and $\hat{N}'$ from their respective subspaces have to commute, $[\hat{B}', \hat{B}] = 0, \dots, [\hat{N}', \hat{N}] = 0$.

2. Separable states

We now address case (2), where the normalization condition

$$\sum_{a,b,\dots,n} |\Psi_{ab\dots n}|^2 = 1 \quad (33)$$

of the probabilities reduces due to the condition, Eq. (25), to

$$|\Psi_{\alpha\beta\dots v}|^2 = 1. \quad (34)$$

With the help of the definition, Eq. (10), of the probability amplitudes, Eq. (34) suggests that, apart from a phase, the state $|a', b', \dots, n'\rangle$ corresponding to the product of measurements $AB \dots N$ is identical to the state $|\Psi\rangle = |\alpha, \beta, \dots, v\rangle$. Hence, a vanishing interference requires that the state $|\Psi\rangle$ is both separable and an eigenstate of the measurement operators $\hat{A}, \hat{B}, \dots, \hat{N}$.

We note that the second requirement can always be met for a separable state by choosing the correct measurement basis. However, for entangled states, this choice is no longer possible.

B. From measurements and states to the interference contribution

In Fig. 2, we summarize the considerations of the previous section in the form of a transit map connecting measurements and states with interference. Here, we distinguish measurements corresponding to commuting and noncommuting operators, and separable and nonseparable states. Moreover, we have to consider a situation where the operators in all subspaces commute or where at least one does not commute.

Likewise, the separable state may or may not be an eigenstate of the measurement defined by the measurement basis.

A given line starting at a measurement and state leads to a prediction of a vanishing or nonvanishing interference term $\mathcal{O}'_I$ defined by Eq. (20). For example, the combination of a measurement of noncommuting operators and an entangled state always leads to a nonvanishing interference. On the other hand, a separable state, which is an eigenstate of the measurement defined by the measurement basis and noncommuting operators, implies a vanishing interference term $\mathcal{O}'_I = 0$.

However, a separable state, which is not an eigenstate of the measurement and commuting operators in at least one subspace but not all, leads to a nonvanishing interference contribution. We note that there exist special cases, as we will show in the next section for the CHSH inequality, where also a vanishing interference contribution can be obtained from this combination of measurements and state.

IV. BIPARTITE SYSTEM: CHSH SCENARIO

In the preceding section, we have shown that the appearance of interference in the probability to obtain a specific measurement outcome in a multipartite system depends on the choice of measurement basis. We now apply these insights to the expectation value $\langle \hat{S} \rangle$ of the CHSH inequality, which involves the sum of four expectation values of combinations of four operators of a bipartite system. In particular, we now demonstrate that, in full analogy to the Hardy scenario [10], the violation of the CHSH inequality requires an interference of probability amplitudes.

A. Classical versus quantum

The CHSH Gedanken experiment [5] consists of two spacelike separated parties, Alice and Bob, who each receive a particle from a common source that prepares a correlated two-particle system. Both sides have to choose one of two possible local measurements on their subsystem, either Q or R for Alice, and S or T for Bob. For all observables Q , R , S , and T , they will measure either $+1$ or -1 as illustrated in Fig. 3.

After repeating the experiment many times, the four expectation values $\langle RS \rangle$, $\langle QS \rangle$, $\langle RT \rangle$, and $\langle QT \rangle$, corresponding to the four possible joint measurements between both parties, are combined in the Bell sum

$$\langle S \rangle \equiv \langle RS \rangle + \langle QS \rangle + \langle RT \rangle - \langle QT \rangle \quad (35)$$

of averages. According to classical physics, the average is bounded [5] above by the inequality

$$|\langle S \rangle| \leq 2. \quad (36)$$

A quantum mechanical description promotes the observables Q , R , S , and T to operators $\hat{Q}$, $\hat{R}$, $\hat{S}$, and $\hat{T}$, and allows the expectation value $\langle \hat{S} \rangle$ to surpass the classical bound [11], that is,

$$|\langle \hat{S} \rangle| \leq 2\sqrt{2}, \quad (37)$$

as long as the state is entangled and the measurement operators do not commute [12].

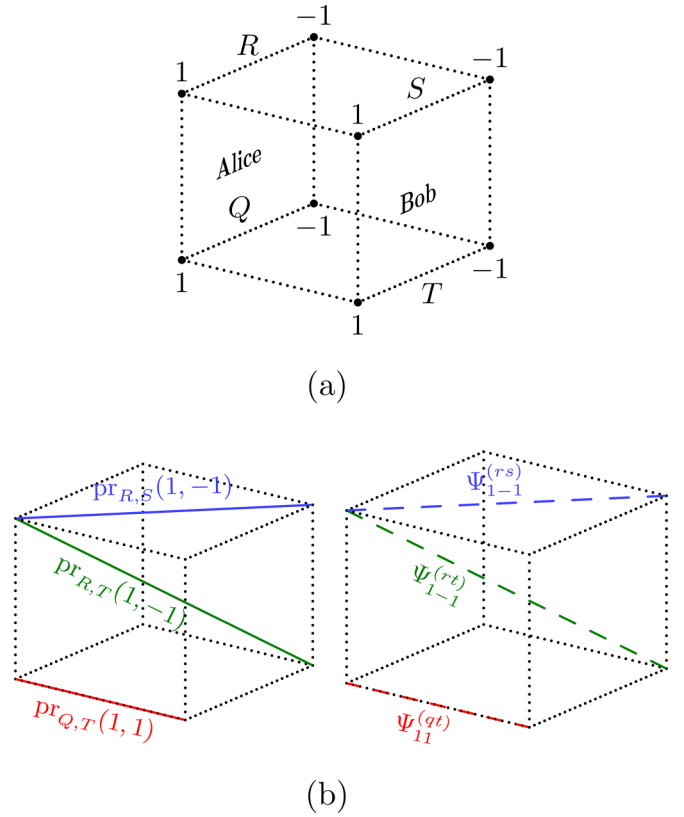


FIG. 3. Classical vs quantum view of the CHSH setup illustrated by a cube whose corners represent the measurement outcomes of Alice and Bob defined by the left and right walls and their connections by classical joint probabilities vs probability amplitudes. The cube in panel (a) is a schematic illustration of the CHSH arrangement, where Alice and Bob each perform one of two possible local measurements on their subsystem. The measurement outcomes $q, r = \pm 1$ for Q or R on Alice's subsystem are located in the four corners of Alice's square. Analogously, the measurement outcomes $s, t = \pm 1$ for S and T on Bob's subsystem are represented by the four corners of Bob's square. Correlations in the system for joint measurements between Alice and Bob connect both planes and make it to a cube. In panel (b), the left cube represents a classical setting, where the connection between two corners of the two opposite planes illustrates the joint probability for Alice and Bob to simultaneously measure a specific outcome, such as the probability $pr_{Q,T}(1, 1)$ (red line) that Alice measures $q = 1$ while Bob measures $t = 1$, the probability $pr_{R,T}(1, -1)$ (green line) that the joint measurement outcome $r = 1$ and $t = -1$ will be observed, and the probability $pr_{R,S}(1, 1)$ (blue line) that Alice and Bob measure R and S with the measurement outcomes $r = 1$ and $s = -1$. The right cube shows a quantum mechanical description of the same examples, where the connection between two corners of the two opposite planes now illustrates probability amplitudes in their respective eigenbases (dashed line).

B. Interfering paths

In order to take advantage of the results of Sec. II, we now identify the operators $\hat{Q}$ and $\hat{R}$ with $\hat{A}'$ and $\hat{A}$, and $\hat{S}$ and $\hat{T}$ with $\hat{B}$ and $\hat{B}'$, respectively. Moreover, we use the eigenbasis $|r, s\rangle$ of $\hat{R}$ and $\hat{S}$ as the measurement basis.

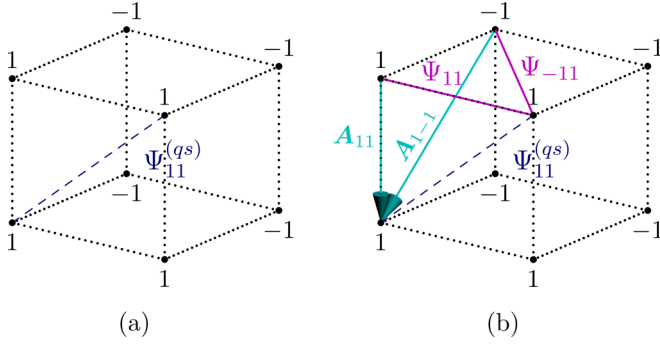


FIG. 4. Probability amplitude represented by interference of possibilities in two different measurement bases. The left cube (a) displays the probability amplitude $\Psi_{11}^{(qs)}$ (dashed line) to measure $q = 1$ and $s = 1$ in the eigenbasis of $\hat{Q}$ and $\hat{S}$. To indicate the basis, we have included q and s as superscripts. The right cube (b) represents $\Psi_{11}^{(qs)}$ in the eigenbasis of $\hat{R}$ and $\hat{S}$, now consisting of two probability amplitudes (purple lines) and matrix elements (blue arrows), such that $\Psi_{11}^{(qs)} = A_{11}\Psi_{11} + A_{-1-1}\Psi_{-1-1}$. For the sake of simplicity, we have suppressed the superscripts r and s on the probability amplitudes Ψ_{11} and Ψ_{-1-1} .

In this case, the expectation value, Eq. (35), reads

$$\begin{aligned} \langle \hat{S} \rangle = & \sum_{r,s} rs |\Psi_{rs}|^2 + \sum_{q,s} qs \left| \sum_r A_{qr} \Psi_{rs} \right|^2 \\ & + \sum_{r,t} rt \left| \sum_s B_{ts} \Psi_{rs} \right|^2 - \sum_{q,t} qt \left| \sum_{r,s} A_{qr} B_{ts} \Psi_{rs} \right|^2, \end{aligned} \quad (38)$$

and the interfering paths that define the probability amplitude to observe a specific measurement outcome in the R - S basis are given by the product of the probability amplitudes $\Psi_{rs} \equiv \langle r, s | \Psi \rangle$ and the matrix elements $A_{qr} \equiv \langle q | r \rangle$ and $B_{ts} \equiv \langle t | s \rangle$.

If the basis transformation is performed in only one of the subspaces, two interfering paths construct the probability amplitude of the measurement outcome, as illustrated for the second term of Eq. (38) in Figs. 4 and 5. However, a transformation in both subspaces results in four interfering paths.

C. No contradiction without interference

In order to connect the violation of the CHSH inequality with interference, we now again decompose the absolute squares in the expectation value $\langle \hat{S} \rangle$, given by Eq. (38), into the two contributions

$$\langle \hat{S} \rangle = S_P + S_I, \quad (39)$$

where S_P consists solely of probabilities and S_I contains all contributions that result from the interference of two or more probability amplitudes. We now show that for $S_I = 0$, the classical bound, Eq. (36), on $\langle \hat{S} \rangle$ cannot be exceeded, leading us to no contradiction. Moreover, we connect the necessary conditions for a vanishing interference contribution with the ones for a violation of the CHSH inequality.

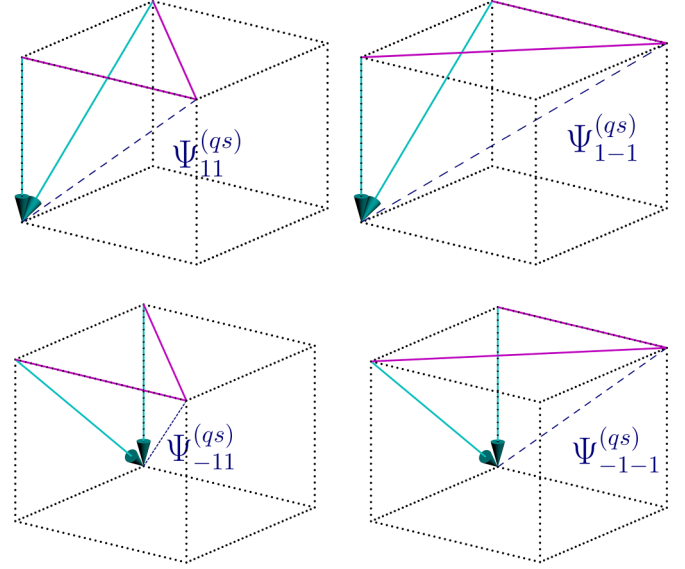


FIG. 5. The four probability amplitudes contributing to the expectation value $\langle \hat{Q} \otimes \hat{S} \rangle$ represented in the eigenbasis of $\hat{R}$ and $\hat{S}$ as interfering paths in four cubes.

1. Vanishing interference defines the classical bound

We first consider the probabilistic term S_P and verify the inequality

$$|S_P| \leq 2. \quad (40)$$

Hence, in order to go beyond the classical bound we need interference.

In order to estimate S_P , we derive in Appendix A an explicit expression for S_P for a specific measurement arrangement. Indeed, for measurements that lie in the x - y plane, the probabilistic contribution

$$S_P = (1 + \cos \Delta_{QR}(1 - \cos \Delta_{TS}) + \cos \Delta_{TS}) \langle \hat{R} \otimes \hat{S} \rangle \quad (41)$$

is ruled by the relative orientations

$$\Delta_{QR} \equiv \vartheta_Q - \vartheta_R \quad (42)$$

and

$$\Delta_{TS} \equiv \vartheta_T - \vartheta_S \quad (43)$$

of the two measurements each party can perform.

The prefactor of the expectation value $\langle \hat{R} \otimes \hat{S} \rangle$ satisfies the inequality

$$-2 \leq 1 + \cos \Delta_{QR}(1 - \cos \Delta_{TS}) + \cos \Delta_{TS} \leq 2, \quad (44)$$

which together with

$$|\langle \hat{R} \otimes \hat{S} \rangle| \leq 1 \quad (45)$$

yields inequality (40).

This derivation relies heavily on the explicit form of S_P . However, we emphasize that the same bounds can be established from the general expression of S_P as shown in Appendix B.

2. Connection to the necessary conditions for a violation

In Sec. III, we have established the conditions for a vanishing interference contribution in a single expectation value $\mathcal{O}_I$, as summarized in Fig. 2. However, the Bell sum $\langle \hat{S} \rangle$ defined by Eq. (35) consists of the sum of four different expectation values. Thus, in order for the interference contribution to vanish, either the interference needs to vanish for all expectation values or the interference contributions need to cancel each other.

The first case is identical to the discussion in Sec. III, summarized by the top of Fig. 2. Below the dashed line in the middle of Fig. 2, we display by the blue line the second possibility where the interference contributions cancel each other.

With the help of the explicit expression

$$\begin{aligned} S_I = & 2[\sin \Delta_{QR}(1 - \cos \Delta_{TS})(\Psi_{11}\Psi_{-11} - \Psi_{-11}\Psi_{-1-1}) \\ & + \sin \Delta_{TS}(1 - \cos \Delta_{QR})(\Psi_{11}\Psi_{1-1} - \Psi_{-11}\Psi_{-1-1}) \\ & - \sin \Delta_{QR} \sin \Delta_{TS}(\Psi_{11}\Psi_{-1-1} + \Psi_{-11}\Psi_{-11})], \end{aligned} \quad (46)$$

for the interference contribution derived in Appendix A, we now discuss these two cases. Here, we have assumed an arbitrary entangled state $|\Psi\rangle$ with real-valued probability amplitudes.

According to Eq. (46), the interference term consists of the sum of three terms, each of which is the product of two contributions, involving measurement angles and probability amplitudes. Hence, the interference term vanishes when in each contribution to the sum, either the factors due to the measurement or those due to the state are zero.

The three combinations of probability amplitudes vanish when all but one of the probability amplitudes Ψ_{rs} with $r, s \in \{-1, 1\}$ are zero. The condition of a vanishing interference contribution arising from the state is thus fully identical to the one discussed in Sec. III, and occurs when the state is separable and an eigenstate of the measurement operators that define the measurement basis. This situation is shown by all lines in Fig. 2 starting from a separable eigenstate leading to a vanishing interference contribution $S_I = 0$ independent of the measurements.

Next, we turn to the terms associated with the measurement shown on the left side of Fig. 2. For commuting operators, that is, for an angle difference $\Delta_{QR} = 0$, corresponding to identical measurement directions as indicated in Fig. 2 below the dashed line by the notation $A \uparrow \uparrow A'$, the interference contribution vanishes independent of the measurement setting Δ_{TS} of the other subsystem. Due to the symmetry of the prefactors in Eq. (46), the same property holds true for $\Delta_{TS} = 0$.

However, for the measurement setting corresponding to the angle difference $\Delta_{QR} = \pi$, which also represents commuting operators but with opposite measurement directions, as indicated in Fig. 2 by the notation $A \uparrow \downarrow A'$, a vanishing interference contribution requires that the measurement setting of the second subsystem has to commute as well, so that $\Delta_{TS} = 0, \pi$. Given that the blue path corresponding to $A \uparrow \downarrow A'$ is connected to a noncommuting measurement in at least one subspace, $\Delta_{TS} \neq 0, \pi$, the interference contribution does not vanish.

We now connect these considerations with the violation of the CHSH inequality: Since a violation requires nonseparability, a state that independent from the measurement arrangement leads to a vanishing interference contribution will never lead to a violation. In other words, all states that do allow for a violation will never yield a vanishing interference contribution $S_I = 0$, unless at least one measurement commutes. Indeed, whenever the interference contribution vanishes due to commuting operators in at least one subspace, the CHSH inequality can no longer be violated since a violation requires noncommutativity of the measurement operators in both subsystems.

In summary, the necessary conditions for a possible violation of the CHSH inequality inevitably lead to a nonvanishing interference contribution to the overall expectation value $\langle \hat{S} \rangle$, without which the classical bounds cannot be surpassed.

D. Example states

So far, we have discussed the theoretical foundations of the interference in the CHSH inequality. In this section, we discuss the role of the probabilistic and the interference contribution in the CHSH case for the example of pure states, as well as the Werner state.

1. Optimal violation of pure states

Any pure two-qubit state can be written in the Schmidt decomposition

$$|\Psi\rangle = \sqrt{\frac{1 + \sqrt{1 - \mathcal{C}^2}}{2}} |01\rangle - \sqrt{\frac{1 - \sqrt{1 - \mathcal{C}^2}}{2}} |10\rangle, \quad (47)$$

where $\mathcal{C}$, with $0 \leq \mathcal{C} \leq 1$, denotes the concurrence. We note that only for $\mathcal{C} = 0$, the state is separable, while for $\mathcal{C} = 1$ the state is maximally entangled.

In Ref. [13], we have derived the optimal measurement directions for a maximal violations of the CHSH inequality. In particular, we have shown that for every $\mathcal{C}$ there exist infinitely many optimal solutions leading to $S = 2\sqrt{1 + \mathcal{C}^2}$. We now investigate the probabilistic $\mathcal{S}_P$, Eq. (41), and interference contributions $S_I = S - \mathcal{S}_P$ for these measurements.

In Appendix C, we show the relations

$$\cos \Delta_{QR} = \frac{(1 - \mathcal{C}^2) \sin \gamma \cos \gamma}{\sqrt{\mathcal{C}^2 + (1 - \mathcal{C}^2)^2 \sin^2 \gamma \cos^2 \gamma}} \quad (48)$$

for the angle Δ_{QR} between the measurement directions of Q and R , and

$$\cos \Delta_{TS} = \frac{1 - \mathcal{C}^2}{1 + \mathcal{C}^2} (\sin^2 \gamma - \cos^2 \gamma) \quad (49)$$

for the angle Δ_{TS} , between T and S . Here, $\gamma \in [0, 2\pi)$ denotes the remaining free parameter when optimizing the violation of the CHSH inequality.

Moreover, the expectation value

$$\langle \hat{R} \otimes \hat{S} \rangle = \frac{\mathcal{C}^2 \cos \gamma \cos(\gamma + \delta) + \sin \gamma \sin(\gamma + \delta)}{\sqrt{\mathcal{C}^2 \cos^2 \gamma + \sin^2 \gamma}} \quad (50)$$

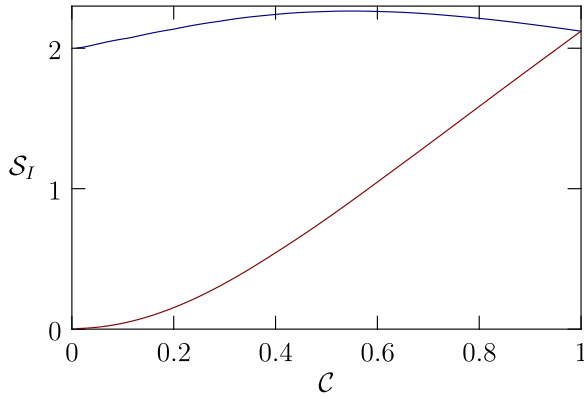


FIG. 6. Minimal (red) and maximal (blue) values of S_I for measurements optimally violating the CHSH inequality as a function of the concurrence $\mathcal{C}$.

of the joint measurement of $\hat{R}$ and $\hat{S}$ involves the angle

$$\delta = \arccot \sqrt{\frac{\mathcal{C}^2 \cos^2 \gamma + \sin^2 \gamma}{\mathcal{C}^2 \sin^2 \gamma + \cos^2 \gamma}}. \quad (51)$$

When we insert these expressions into the probabilistic contribution, Eq. (41), for an arbitrary concurrence $\mathcal{C}$, the probabilistic $\mathcal{S}_P$ and thus also the interference contribution S_I depend on the parameter γ . Hence, for a given concurrence, the measurements leading to a maximal violation of the CHSH inequality have different probabilistic and interference contributions, depending on the measurement setting, represented by γ . We note that different values of γ can also be achieved by keeping the measurement setting but changing the basis from R - S to a different basis.

In Fig. 6, we depict the maximal and minimal values of the interference contribution S_I as a function of the concurrence $\mathcal{C}$. For small concurrences, the possible values of S_I exhibit a large range, while for larger concurrences this range decreases. In the special case of a separable state, the entire value of the Bell sum $\mathcal{S} = 2$ results from either the probabilistic contribution ($S_I = 0$) or the interference contribution ($S_I = 2$).

We note that while the minimal interference contribution is monotonically increasing with the concurrence, this behavior is not true for the maximal interference contribution. Indeed, our numerical analysis shows that the interference contribution reaches its maximal value for $\mathcal{C} \approx 0.55$.

For a maximally entangled state, that is, $\mathcal{C} = 1$, Eqs. (48) and (50) simplify to $\cos \Delta_{QR} = \cos \Delta_{TS} = 0$ and $\langle \hat{R} \otimes \hat{S} \rangle = 1/\sqrt{2}$, and thus $\mathcal{S}_P = 1/\sqrt{2}$, which is independent of the choice of the measurement basis. We note that the probabilistic contribution is not given by the classical bound of $\mathcal{S} = 2$, and the interference is larger than the violation of the CHSH bound.

2. Werner states

While we have only considered pure states for the investigation of the probabilistic and interference contributions entering the expectation value $\langle \hat{S} \rangle$, the concept of the separation of both contributions can be adapted easily to statistical

mixtures of states. We illustrate this concept for the Werner state [14]

$$\hat{\Psi}_W = p |\Psi^-\rangle \langle \Psi^-| + \frac{1-p}{4} \hat{\mathbb{1}}, \quad (52)$$

consisting of a mixture of an inseparable maximally entangled state $|\Psi^-\rangle \langle \Psi^-|$ and a separable maximally mixed state $\hat{\mathbb{1}}/4$, with statistical weight $0 < p < 1$. The Werner state has the property that while it is nonseparable for weights $p > 1/3$ [15,16], a violation of the CHSH inequality can only be achieved if, in addition, the weight exceeds the value $p > 1/\sqrt{2}$.

Hence, the Bell sum $\hat{\mathcal{S}}$ for the Werner state reads

$$\langle \hat{\mathcal{S}} \rangle_{\Psi_W} = p \langle \hat{\mathcal{S}} \rangle_{\Psi^-} + \frac{1-p}{4} \langle \hat{\mathcal{S}} \rangle_{\hat{\mathbb{1}}}. \quad (53)$$

Since the first contribution of the mixture corresponds to the pure state, the expectation value $\langle \hat{\mathcal{S}} \rangle_{\Psi^-}$ allows the decomposition

$$\langle \hat{\mathcal{S}} \rangle_{\Psi^-} = \mathcal{S}_P^{(\Psi^-)} + S_I^{(\Psi^-)}, \quad (54)$$

as already shown before.

For the second contribution that corresponds to a mixed but separable state of the form $\Psi = \sum_i p_i |\Psi_i\rangle \langle \Psi_i|$ with $|\Psi_i\rangle = |j\rangle \otimes |k\rangle$ being a bipartite state, the expectation value

$$\langle \hat{\mathcal{S}} \rangle_{\Psi} = \sum_i p_i \text{Tr}(\hat{\mathcal{S}} |\Psi_i\rangle \langle \Psi_i|) \quad (55)$$

reads

$$\langle \hat{\mathcal{S}} \rangle_{\Psi} = \sum_i p_i \langle \hat{\mathcal{S}} \rangle_{\Psi_i}, \quad (56)$$

which again, in the exact manner as before, splits into the two contributions

$$\langle \hat{\mathcal{S}} \rangle = \sum_i p_i (\mathcal{S}_P^{(i)} + S_I^{(i)}). \quad (57)$$

If, for example, we now again restrict our measurement configurations to the x - y plane and substitute Eq. (41) into the probabilistic contribution

$$\mathcal{S}_P = \sum_i p_i \mathcal{S}_P^{(i)}, \quad (58)$$

we arrive at

$$\mathcal{S}_P = (1 + \cos \Delta_{QR}(1 - \cos \Delta_{TS}) + \cos \Delta_{TS}) \text{Tr}(\hat{R} \otimes \hat{S} \Psi). \quad (59)$$

For the Werner state, where $\Psi = \hat{\mathbb{1}}/4$, we find the identity

$$\text{Tr}(\hat{R} \otimes \hat{S}) = 0, \quad (60)$$

since any general measurement in the x - y plane is described by Pauli operators.

Hence, the probabilistic contribution $\mathcal{S}_P = 0$ vanishes. It is clear that, in this case, the interference contribution S_I needs to vanish too, given that the expectation value

$$\langle \hat{\mathcal{S}} \rangle_{\hat{\mathbb{1}}} = 0 \quad (61)$$

of the second contribution to the Werner state vanishes.

Hence, the interference contribution of the Werner state

$$\mathcal{S}_I^{(\Psi_W)} = p \mathcal{S}_I^{(\Psi^-)} \quad (62)$$

is just the scaled interference contribution of the maximally entangled state, due to the linearity of the state and the vanishing interference contribution of the maximally mixed state. Therefore, the interference contribution does not vanish except for $p = 0$, which is a maximally mixed state. As a result, the probabilistic and interference contributions do not provide a deeper insight into at the range $1/3 \leq p \leq 1/\sqrt{2}$ for which the state is entangled, but cannot violate the CHSH inequality.

V. MULTIPARTITE SYSTEM: GHZ SCENARIO

In our second example, illustrating the inner workings of interference, we now focus on a multipartite system consisting of three particles on which Alice, Bob, and Charlie perform measurements. The GHZ setup [9] considers four expectation values of joint measurements of three operators. In this section, we show that these expectation values leading to a contradiction to classical physics arise solely from interference; that is, the corresponding probabilistic contributions vanish. In order to focus on the essential steps of the derivation, we concentrate on only two expectation values. The analysis for the other two is identical to this one.

For our argument, we select the expectation values

$$\mathcal{O}_3 \equiv \langle \hat{A} \otimes \hat{B} \otimes \hat{C} \rangle \equiv \langle \hat{\sigma}_x \otimes \hat{\sigma}_x \otimes \hat{\sigma}_x \rangle \quad (63)$$

and

$$\mathcal{O}'_3 \equiv \langle \hat{A}' \otimes \hat{B}' \otimes \hat{C}' \rangle \equiv \langle \hat{\sigma}_x \otimes \hat{\sigma}_y \otimes \hat{\sigma}_y \rangle, \quad (64)$$

where we have recalled the notation of Sec. II, and $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ denote the Pauli matrices.

Next, we represent the three operators $\hat{A}'$, $\hat{B}'$, and $\hat{C}'$ in the eigenbasis of the measurement operators $\hat{A}$, $\hat{B}$, and $\hat{C}$, and arrive at the expression

$$\mathcal{O}'_3 = \sum_{a',b',c'} a' b' c' \left| \sum_{a,b,c} \mathbf{A}_{a'a} \mathbf{B}_{b'b} \mathbf{C}_{c'c} \Psi_{abc} \right|^2. \quad (65)$$

In complete analogy to the previous sections, we now analyze the decomposition

$$\mathcal{O}'_3 = \mathcal{O}'_p + \mathcal{O}'_I \quad (66)$$

of $\mathcal{O}'_3$ into the probabilistic contribution

$$\mathcal{O}'_p = \sum_{a',b',c'} a' b' c' \sum_{a,b,c} |\mathbf{A}_{a'a}|^2 |\mathbf{B}_{b'b}|^2 |\mathbf{C}_{c'c}|^2 |\Psi_{abc}|^2, \quad (67)$$

containing only the absolute squares and the interference contribution $\mathcal{O}'_I$.

In order to determine the elements of the matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$, given by Eq. (9), we first note that $\hat{A}' = \hat{A} = \hat{\sigma}_x$, and thus the matrix

$$\mathbf{A} = \hat{\mathbb{1}} \quad (68)$$

is trivial.

Moreover, since $\hat{B}' = \hat{C}' = \hat{\sigma}_y$ and $\hat{B} = \hat{C} = \hat{\sigma}_x$, the two matrices $\mathbf{B}$ and $\mathbf{C}$ are identical. As a result, it suffices to focus

on $\mathbf{B}$, whose matrix elements are given by

$$\mathbf{B}_{b'b} = \langle y_{b'} | x_b \rangle \quad (69)$$

with eigenvalues $b', b = \pm 1$, corresponding to the eigenvectors $|x_b\rangle$ and $|y_{b'}\rangle$ of $\hat{\sigma}_x$ and $\hat{\sigma}_y$, respectively.

The absolute value squared of the scalar product between these eigenvectors reads

$$|\langle y_{b'} | x_b \rangle|^2 = |\langle y_{b'} | \hat{\sigma}_y \hat{\sigma}_x | x_b \rangle|^2 = |\langle y_{b'} | \hat{\sigma}_z | x_b \rangle|^2, \quad (70)$$

and with the help of the identities

$$\hat{\sigma}_z |x_b\rangle = |x_{-b}\rangle \quad (71)$$

and

$$\langle y_{b'} | \hat{\sigma}_z = \langle y_{-b'} |, \quad (72)$$

we obtain

$$|\langle y_{b'} | x_b \rangle|^2 = |\langle y_{b'} | x_{-b} \rangle|^2 \quad (73)$$

and

$$|\langle y_{b'} | x_b \rangle|^2 = |\langle y_{-b'} | x_b \rangle|^2. \quad (74)$$

Hence, the absolute value squared of the matrix elements

$$|\mathbf{B}_{b',b}|^2 = k \quad (75)$$

is independent of the indices b' and b , and given by a constant k .

Since the two matrices $\mathbf{B}$ and $\mathbf{C}$ are identical, we also find

$$|\mathbf{C}_{c',c}|^2 = k. \quad (76)$$

When we insert Eqs. (68), (75), and (76) into our expression, Eq. (67), for $\mathcal{O}'_p$ we arrive at

$$\mathcal{O}'_p = \sum_{a,b,c} a |\Psi_{abc}|^2 k^2 \sum_{b'} b' \sum_{c'} c'. \quad (77)$$

Due to the eigenvalues $b', c' = \pm 1$, the summations over b' and c' vanish, that is,

$$\sum_{b'} b' = \sum_{c'} c' = 0, \quad (78)$$

leading us to a vanishing probabilistic contribution

$$\mathcal{O}'_p = 0. \quad (79)$$

Thus, we find from the decomposition, Eq. (66), of the expectation value $\mathcal{O}'_3$ into the probabilistic and interference contribution the identity

$$\mathcal{O}'_3 = \mathcal{O}'_I, \quad (80)$$

demonstrating that $\mathcal{O}'_3$ is entirely built up by the interference contribution.

Moreover, for a perfectly correlated three-particle state

$$|\Psi\rangle \equiv \frac{1}{\sqrt{2}}(|0, 0, 0\rangle + |1, 1, 1\rangle), \quad (81)$$

we obtain from the definition, Eq. (82), of $\mathcal{O}'_3$ the relation

$$\mathcal{O}'_3 = -1 = \mathcal{O}'_I \quad (82)$$

indicating that the nonvanishing expectation value $\mathcal{O}'_3$ is solely due to interference.

So far, we have only considered two of the four expectation values. The other two,

$$\mathcal{O}_3'' \equiv \langle \hat{\sigma}_y \otimes \hat{\sigma}_x \otimes \hat{\sigma}_y \rangle, \quad (83a)$$

$$\mathcal{O}_3''' \equiv \langle \hat{\sigma}_y \otimes \hat{\sigma}_y \otimes \hat{\sigma}_x \rangle, \quad (83b)$$

involve again only $\hat{\sigma}_x$ and $\hat{\sigma}_y$.

For this reason, an identical derivation yields

$$\mathcal{O}_3'' = \mathcal{O}_I'' = -1, \quad (84a)$$

$$\mathcal{O}_3''' = \mathcal{O}_I''' = -1. \quad (84b)$$

We emphasize that this asymmetric distribution between $\mathcal{O}_p'$ and $\mathcal{O}_I'$ favoring interference results from our choice of the measurement basis. In a different measurement basis, the distribution between both contributions is less asymmetric.

We conclude by noting that, in contrast to the analysis of the CHSH inequality, the GHZ situation seems much more elementary. Indeed, it results from the fact that the absolute value squares of the elements of two matrices are constant, and the sum, Eq. (78), over the eigenvalues vanishes.

VI. CONCLUSIONS AND OUTLOOK

Motivated by the necessity of destructive interference [10] for a contradiction between a classical and a quantum mechanical description of the Hardy scenario, we have revisited the role of interference in quantum correlations. In particular, we have shown that the expectation value of Hermitian operators for a general n -partite system contains interference, provided the measurement basis is not the eigenbasis of the operators. Moreover, we have found necessary conditions for a nonvanishing interference. Interestingly enough, those conditions are intertwined with the necessary conditions to achieve a violation of the CHSH inequality.

Indeed, interference in an expectation value, or more precisely in probabilities, only vanishes in two situations: (1) whenever the measurement operator commutes with another measurement operator that sets the measurement basis or (2) whenever the state is separable and an eigenstate of the operator defining the measurement basis. Consequently, the necessary requirement of noncommutativity and entanglement in order to achieve a possible violation of the CHSH inequality can no longer be met.

In addition, we have verified for the special case of the CHSH inequality that the probabilistic contribution $\mathcal{S}_p$ lies within the classical bounds. Hence, it is interference that enables a violation of the CHSH inequality.

The interference picture introduced for general multipartite systems and illustrated by the CHSH inequality also applies to the GHZ experiment. Again, we find interference at the core of the violation of classical concepts.

We note that although the presence of interference is necessary to find a violation of classical predictions, we have also shown that it is not sufficient. Even for a separable state, the right basis choice allows us to formulate the result as an interference contribution. This behavior is in total agreement with the results of Ref. [17], where different interference

phenomena were explained by a classical toy model, while certain predictions of quantum mechanics, such as the violation of Bell inequalities, could not be explained by this model. The question whether there exists a sufficiency criterion for interference predicting a nonclassical result remains an interesting problem for future considerations.

Another interesting question along this line regards the role of interference for sets of incompatible measurements that never lead to bipartite Bell violations, although they reveal multipartite Bell nonlocality [18]. For such measurements, either the interference is always present, even though no violation for a bipartite Bell inequality can be found, or the interference vanishes in a bipartite case but not in the multipartite scenario. In the first case, it would be interesting to investigate why this interference contribution is not sufficient to violate a Bell inequality, while in the second case a better understanding of the vanishing interference could shed light onto the multipartite entangled systems. Unfortunately, a full evaluation of this question goes beyond the scope of this article.

Throughout this article, we have focused on pure states and projective measurements. However, as shown by the example of the Werner state, our formalism can easily be extended to mixed states. In the same way, an extension to positive operator-valued measures (POVMs) is possible. Indeed, it is known [19] that there exist noncommuting observables such as $\hat{M}_x \equiv (\hat{1} + \lambda_x \hat{\sigma}_x)/2$ and $\hat{M}_z \equiv (\hat{1} + \lambda_z \hat{\sigma}_z)/2$, which for $\lambda_x^2 + \lambda_z^2 < 1$ lead to compatible measurements. Our results suggest that for these measurements the interference contribution is proportional to the parameters λ_x and λ_z , and thus decreases for decreasing λ_x and λ_z . However, similar to the Werner states, where interference is present even for separable states, we expect the interference contribution to still be present even in the compatible measurement regime. Needless to say, a more detailed analysis has to await a future publication.

While our formalism has revealed a deeper connection between nonlocality measures and quantum interference, at first sight, our results do not seem to lead to new experimental tests of quantum mechanics. However, at least two ideas to take advantage of our insights for a step in this direction offer themselves.

By separating the probabilistic contribution from the interference part, we directly have access to the classical bounds. Thus, by reverse engineering of our formalism, and starting from the probabilistic contribution, we might identify measurements that increase the interference contribution beyond these probabilistic limits, leading to new experimental arrangements for nonlocality measures.

Moreover, quantum theory provides limits on nonlocality measures, which often do not coincide with the most general ones possible. For instance, the Tsirelson bound $2\sqrt{2}$ for the CHSH case is far below the value 4 of a completely generalized nonlocal probability theory. Since we identify interference as the key ingredient in nonlocality measures, such quantum mechanical boundaries are therefore set by interference.

We are confident that our approach will provide a deeper insight into the bounds of quantum theory and its comparison to any probabilistic nonlocal theory.

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DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: CHSH EXPECTATION VALUE: EXPLICIT EXPRESSIONS FOR THE PROBABILISTIC AND INTERFERENCE CONTRIBUTIONS

In this Appendix, we derive explicit expressions for the probabilistic and interference contributions, $\mathcal{S}_P$ and $\mathcal{S}_I$, to the CHSH expectation value

$$\begin{aligned} \langle \hat{S} \rangle = & \sum_{r,s} rs |\Psi_{rs}|^2 + \sum_{q,s} qs \left| \sum_r \mathbf{A}_{qr} \Psi_{rs} \right|^2 \\ & + \sum_{r,t} rt \left| \sum_s \mathbf{B}_{ts} \Psi_{rs} \right|^2 - \sum_{q,t} qt \left| \sum_{r,s} \mathbf{A}_{qr} \mathbf{B}_{ts} \Psi_{rs} \right|^2. \end{aligned} \quad (\text{A1})$$

We start by first obtaining the matrix elements $\mathbf{A}_{qr}$ and $\mathbf{B}_{ts}$ for a specific basis, and then obtain formulas for $\mathcal{S}_P$ and $\mathcal{S}_I$.

1. Matrix elements

We describe general measurements $\hat{U} \in \{\hat{Q}, \hat{R}\}$ for Alice and $\hat{V} \in \{\hat{S}, \hat{T}\}$ for Bob by measurement operators

$$\hat{U} \equiv \mathbf{u} \cdot \hat{\boldsymbol{\sigma}} \quad (\text{A2})$$

and

$$\hat{V} \equiv \mathbf{v} \cdot \hat{\boldsymbol{\sigma}}, \quad (\text{A3})$$

described by three-dimensional real-valued unit vectors $\mathbf{u} \equiv (\cos \varphi_U \cos \vartheta_U, \sin \varphi_U \cos \vartheta_U, \sin \vartheta_U)^T$ and $\mathbf{v} \equiv (\cos \varphi_V \cos \vartheta_V, \sin \varphi_V \cos \vartheta_V, \sin \vartheta_V)^T$ with azimuthal angles $\varphi_U, \varphi_V \in [0, 2\pi]$ and polar angles $\vartheta_U, \vartheta_V \in [-\pi/2, \pi/2]$ that set the measurement direction, and the vector $\hat{\boldsymbol{\sigma}}$ formed by the Pauli matrices.

For simplicity, we restrict the measurements to the x - y plane and thus set $\varphi_U = 0$ and $\varphi_V = 0$. The eigenvectors of the measurement operators for Alice

$$\hat{U} = \begin{pmatrix} \sin \vartheta_U & \cos \vartheta_U \\ \cos \vartheta_U & -\sin \vartheta_U \end{pmatrix} \quad (\text{A4})$$

and Bob

$$\hat{V} = \begin{pmatrix} \sin \vartheta_V & \cos \vartheta_V \\ \cos \vartheta_V & -\sin \vartheta_V \end{pmatrix} \quad (\text{A5})$$

are given by

$$|j = 1\rangle = \sin\left(\frac{\pi}{4} - \frac{\vartheta_J}{2}\right) |0\rangle - \cos\left(\frac{\pi}{4} - \frac{\vartheta_J}{2}\right) |1\rangle \quad (\text{A6})$$

corresponding to the eigenvalue $j = 1$ and

$$|j = -1\rangle = \cos\left(\frac{\pi}{4} - \frac{\vartheta_J}{2}\right) |0\rangle + \sin\left(\frac{\pi}{4} - \frac{\vartheta_J}{2}\right) |1\rangle \quad (\text{A7})$$

corresponding to the eigenvalue $j = -1$ for $j \in \{u, v\}$, with $J \in \{U, V\}$.

When we substitute them into the definition, Eq. (9), of the matrix elements $\mathbf{A}_{qr}$ and $\mathbf{B}_{ts}$, we obtain the matrices

$$\mathbf{A} = \begin{pmatrix} \cos \frac{\Delta_{QR}}{2} & \sin \frac{\Delta_{QR}}{2} \\ -\sin \frac{\Delta_{QR}}{2} & \cos \frac{\Delta_{QR}}{2} \end{pmatrix} \quad (\text{A8})$$

and

$$\mathbf{B} = \begin{pmatrix} \cos \frac{\Delta_{TS}}{2} & \sin \frac{\Delta_{TS}}{2} \\ -\sin \frac{\Delta_{TS}}{2} & \cos \frac{\Delta_{TS}}{2} \end{pmatrix}, \quad (\text{A9})$$

where we have defined the angle differences $\Delta_{QR} \equiv \vartheta_Q - \vartheta_R$ and $\Delta_{TS} \equiv \vartheta_T - \vartheta_S$.

2. Probabilistic contribution

In order to find an explicit expression for the probabilistic contribution

$$\begin{aligned} \mathcal{S}_P \equiv & \sum_{r,s} rs |\Psi_{rs}|^2 + \sum_{r,q,s} qs |\mathbf{A}_{qr}|^2 |\Psi_{rs}|^2 \\ & + \sum_{s,r,t} rt |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 - \sum_{r,s,t,q} qt |\mathbf{A}_{qr}|^2 |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 \end{aligned} \quad (\text{A10})$$

of the Bell sum, Eq. (35), we first note that the first term of Eq. (A10) is the definition of the expectation value

$$\langle \hat{R} \otimes \hat{S} \rangle \equiv \sum_{r,s} rs |\Psi_{rs}|^2 \quad (\text{A11})$$

of the joint measurement of $\hat{R}$ and $\hat{S}$.

From the explicit representation, Eq. (A8), of the matrix $\mathbf{A}$, we find the expression

$$|\mathbf{A}_{qr}|^2 = \delta_{q,r} \cos^2 \frac{\Delta_{QR}}{2} + \delta_{q,-r} \sin^2 \frac{\Delta_{QR}}{2} \quad (\text{A12})$$

for the absolute value squared of the matrix elements $\mathbf{A}_{qr}$, which when inserted into the second term of Eq. (A10) leads us to

$$\sum_{r,q,s} qs |\mathbf{A}_{qr}|^2 |\Psi_{rs}|^2 = \sum_{r,s} rs \left[\cos^2 \frac{\Delta_{QR}}{2} - \sin^2 \frac{\Delta_{QR}}{2} \right] |\Psi_{rs}|^2, \quad (\text{A13})$$

where we have already performed the summation over the index q .

When we use the trigonometric identity

$$\cos x \equiv \cos^2 \frac{x}{2} - \sin^2 \frac{x}{2} \quad (\text{A14})$$

together with the expectation value, Eq. (A11), for the joint $\hat{R}$ and $\hat{S}$ measurement, we find

$$\sum_{r,q,s} qs |\mathbf{A}_{qr}|^2 |\Psi_{rs}|^2 = \cos \Delta_{QR} \langle \hat{R} \otimes \hat{S} \rangle. \quad (\text{A15})$$

Analogously, we use the relation

$$|B_{ts}|^2 = \delta_{t,s} \cos^2 \frac{\Delta_{TS}}{2} + \delta_{t,-s} \sin^2 \frac{\Delta_{TS}}{2} \quad (\text{A16})$$

for the absolute value squared of the matrix elements $\mathbf{B}_{ts}$ and obtain the expression

$$\sum_{s,r,t} rt |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 = \cos \Delta_{TS} \langle \hat{R} \otimes \hat{S} \rangle \quad (\text{A17})$$

for the third term of Eq. (A10).

Finally, we use the representations, Eqs. (A12) and (A16), of the matrix elements together with our trigonometric identity, Eq. (A14), and the joint expectation value $\langle \hat{R} \otimes \hat{S} \rangle$, Eq. (A11), and find that the last term of Eq. (A10) is given by

$$\sum_{r,s,t,q} qt |\mathbf{A}_{qr}|^2 |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 = \cos \Delta_{QR} \cos \Delta_{TS} \langle \hat{R} \otimes \hat{S} \rangle. \quad (\text{A18})$$

Hence, the probabilistic contribution

$$S_P = (1 + \cos \Delta_{QR} + \cos \Delta_{TS} - \cos \Delta_{QR} \cos \Delta_{TS}) \langle \hat{R} \otimes \hat{S} \rangle \quad (\text{A19})$$

to the Bell sum depends only on the angle differences Δ_{QR} and Δ_{TS} and the expectation value of the joint $\hat{R}$ and $\hat{S}$ measurement.

3. Interference contribution

Next, we address the interference contribution

$$S_I \equiv I_1 + I_2 - I_3, \quad (\text{A20})$$

where we have introduced the abbreviations

$$I_1 \equiv \sum_{q,s} qs \sum_{(r \neq \tilde{r})} \mathbf{A}_{qr} \mathbf{A}_{q\tilde{r}}^* \Psi_{rs} \Psi_{r\tilde{s}}^* \quad (\text{A21})$$

and

$$I_2 \equiv \sum_{r,t} rt \sum_{(s \neq \tilde{s})} \mathbf{B}_{ts} \mathbf{B}_{t\tilde{s}}^* \Psi_{rs} \Psi_{r\tilde{s}}^*, \quad (\text{A22})$$

as well as

$$I_3 \equiv \sum_{q,t} qt \sum_{(r,s) \neq (\tilde{r},\tilde{s})} \mathbf{A}_{qr} \mathbf{A}_{q\tilde{r}}^* \mathbf{B}_{ts} \mathbf{B}_{t\tilde{s}}^* \Psi_{rs} \Psi_{r\tilde{s}}^*. \quad (\text{A23})$$

From Eq. (A8), we note that the matrix elements $\mathbf{A}_{qr}$ are real and satisfy the properties $\mathbf{A}_{11} = \mathbf{A}_{-1-1}$ and $\mathbf{A}_{-11} = -\mathbf{A}_{1-1}$. When we further use the condition $z + z^* = 2 \operatorname{Re} z$ for an arbitrary complex number z , we find

$$I_1 = 4\mathbf{A}_{11}\mathbf{A}_{-1-1} \operatorname{Re}(\Psi_{11}\Psi_{-11}^* - \Psi_{-1-1}\Psi_{11}^*), \quad (\text{A24})$$

which with the explicit form of the matrix elements reduces to

$$I_1 = 2 \sin \Delta_{QR} \operatorname{Re}(\Psi_{11}\Psi_{-11}^* - \Psi_{-1-1}\Psi_{11}^*). \quad (\text{A25})$$

Similarly, we obtain from the definition, Eq. (A9), of $\mathbf{B}_{ts}$ with the help of the symmetry relations $\mathbf{B}_{11} = \mathbf{B}_{-1-1}$ and $\mathbf{B}_{-11} = -\mathbf{B}_{1-1}$ the representation

$$I_2 = 4\mathbf{B}_{11}\mathbf{B}_{1-1} \operatorname{Re}(\Psi_{11}\Psi_{1-1}^* - \Psi_{-11}\Psi_{-1-1}^*) \quad (\text{A26})$$

or

$$I_2 = 2 \sin \Delta_{TS} \operatorname{Re}(\Psi_{11}\Psi_{1-1}^* - \Psi_{-11}\Psi_{-1-1}^*). \quad (\text{A27})$$

Likewise, we derive

$$\begin{aligned} I_3 &= 8\mathbf{A}_{1-1}\mathbf{A}_{11}\mathbf{B}_{11}\mathbf{B}_{1-1} \operatorname{Re}(\Psi_{11}\Psi_{-1-1}^* - \Psi_{-1-1}\Psi_{11}^*) \\ &\quad + 4(|\mathbf{A}_{11}|^2 - |\mathbf{A}_{-11}|^2)\mathbf{B}_{11}\mathbf{B}_{1-1} \\ &\quad \times \operatorname{Re}(\Psi_{11}\Psi_{1-1}^* - \Psi_{-11}\Psi_{-1-1}^*) + 4\mathbf{A}_{11}\mathbf{A}_{1-1}(|\mathbf{B}_{11}|^2 \\ &\quad - |\mathbf{B}_{-11}|^2) \operatorname{Re}(\Psi_{11}\Psi_{-11}^* - \Psi_{-1-1}\Psi_{-1-1}^*) \end{aligned} \quad (\text{A28})$$

or explicitly

$$\begin{aligned} I_3 &= 2[\sin \Delta_{QR} \sin \Delta_{TS} \operatorname{Re}(\Psi_{11}\Psi_{-1-1}^* - \Psi_{-1-1}\Psi_{11}^*) \\ &\quad + \cos \Delta_{QR} \sin \Delta_{TS} \operatorname{Re}(\Psi_{11}\Psi_{1-1}^* - \Psi_{-11}\Psi_{-1-1}^*) \\ &\quad + \sin \Delta_{QR} \cos \Delta_{TS} \operatorname{Re}(\Psi_{11}\Psi_{-11}^* - \Psi_{-1-1}\Psi_{-1-1}^*)]. \end{aligned} \quad (\text{A29})$$

When we substitute Eqs. (A25), (A27), and (A29) into the interference contribution, Eq. (A20), and rearrange the terms, we finally find the explicit expression

$$\begin{aligned} S_I &= 2[\sin \Delta_{QR}(1 - \cos \Delta_{TS}) \operatorname{Re}(\Psi_{11}\Psi_{-11}^* - \Psi_{-1-1}\Psi_{-1-1}^*) \\ &\quad + \sin \Delta_{TS}(1 - \cos \Delta_{QR}) \operatorname{Re}(\Psi_{11}\Psi_{1-1}^* - \Psi_{-11}\Psi_{-1-1}^*) \\ &\quad - \sin \Delta_{QR} \sin \Delta_{TS} \operatorname{Re}(\Psi_{11}\Psi_{-1-1}^* + \Psi_{-1-1}\Psi_{-11}^*)] \end{aligned} \quad (\text{A30})$$

for a general measurement.

APPENDIX B: BOUND OF THE PROBABILISTIC CONTRIBUTION

In this Appendix, we show that the values of the probabilistic contribution

$$\begin{aligned} S_P &\equiv \sum_{r,s} rs |\Psi_{rs}|^2 + \sum_{r,q,s} qs |\mathbf{A}_{qr}|^2 |\Psi_{rs}|^2 \\ &\quad + \sum_{s,r,t} rt |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 - \sum_{r,s,t,q} qt |\mathbf{A}_{qr}|^2 |\mathbf{B}_{ts}|^2 |\Psi_{rs}|^2 \end{aligned} \quad (\text{B1})$$

of the Bell sum are restricted by the classical bound, Eq. (36), of the CHSH inequality. We emphasize that our derivation relies on the triangle inequality and does not take advantage of the explicit expressions of the matrix elements $\mathbf{A}_{qr}$ and $\mathbf{B}_{ts}$.

For this purpose, we first rearrange the contributions to S_P into a product of terms that contain only the matrix elements $\mathbf{A}_{qr}$ and $\mathbf{B}_{ts}$ connecting the two sets of measurement operators, and the probability amplitude Ψ_{rs} of the state in the R - S basis,

$$S_P = \sum_{r,s} [\tilde{q}_r(s - \tilde{t}_s) + r(s + \tilde{t}_s)] |\Psi_{rs}|^2. \quad (\text{B2})$$

Here, we have introduced the abbreviations

$$\tilde{q}_r \equiv \sum_q q |\mathbf{A}_{qr}|^2 \quad (\text{B3})$$

as well as

$$\tilde{t}_s \equiv \sum_t t |\mathbf{B}_{ts}|^2. \quad (\text{B4})$$

Next, we use the triangle inequality, which shows that the absolute value of $\mathcal{S}_P$ is bounded from above by

$$|\mathcal{S}_P| \leq \sum_{r,s} |\tilde{q}_r(s - \tilde{t}_s) + r(s + \tilde{t}_s)| |\Psi_{rs}|^2, \quad (\text{B5})$$

which again with the help of the triangle inequality leads us to

$$|\mathcal{S}_P| \leq \sum_{r,s} [|\tilde{q}_r||s - \tilde{t}_s| + |r||s + \tilde{t}_s|] |\Psi_{rs}|^2. \quad (\text{B6})$$

From the definition, Eq. (B3), we find the inequality

$$|\tilde{q}_r| = ||\mathbf{A}_{1r}|^2 - |\mathbf{A}_{-1r}|^2| \leq \max(|\mathbf{A}_{1r}|^2, |\mathbf{A}_{-1r}|^2), \quad (\text{B7})$$

which together with the unitary property of $\mathbf{A}$ yields

$$|\tilde{q}_r| \leq 1. \quad (\text{B8})$$

With $|r| = 1$, we find the upper bound

$$|\mathcal{S}_P| \leq \sum_{r,s} [|s - \tilde{t}_s| + |s + \tilde{t}_s|] |\Psi_{rs}|^2, \quad (\text{B9})$$

which with the identity

$$|s - \tilde{t}_s| + |s + \tilde{t}_s| = 2 \max(|s|, |\tilde{t}_s|) \quad (\text{B10})$$

reads

$$|\mathcal{S}_P| \leq 2 \sum_{r,s} \max(|s|, |\tilde{t}_s|) |\Psi_{rs}|^2. \quad (\text{B11})$$

In complete analogy to the estimate, Eq. (B7), of $|\tilde{q}_r|$, we obtain from the definition, Eq. (B4), and the unitarity of $\mathbf{B}$ the inequality

$$|\tilde{t}_s| \leq 1, \quad (\text{B12})$$

and arrive with $|s| = 1$ at

$$|\mathcal{S}_P| \leq 2 \sum_{r,s} |\Psi_{rs}|^2 = 2, \quad (\text{B13})$$

where in the last step we have used the normalization of probabilities.

APPENDIX C: MEASUREMENTS FOR A MAXIMAL VIOLATION OF THE CHSH INEQUALITY

In this Appendix, we derive expressions for the angles Δ_{QR} and Δ_{TS} , as well as the expectation value $\langle \hat{R} \otimes \hat{S} \rangle$ for the measurements that maximally violate the CHSH inequality for a pure state with concurrence $\mathcal{C}$.

We start by recalling from Ref. [13] that optimal measurement directions are given by

$$\mathbf{q} = \mp \frac{1}{\sqrt{\mathcal{C}^2 \sin^2 \gamma + \cos^2 \gamma}} \begin{pmatrix} -\mathcal{C} \cos \theta \sin \gamma \\ -\mathcal{C} \sin \theta \sin \gamma \\ \cos \gamma \end{pmatrix} \quad (\text{C1})$$

and

$$\mathbf{r} = \mp \frac{1}{\sqrt{\mathcal{C}^2 \cos^2 \gamma + \sin^2 \gamma}} \begin{pmatrix} \mathcal{C} \cos \theta \cos \gamma \\ \mathcal{C} \sin \theta \cos \gamma \\ \sin \gamma \end{pmatrix} \quad (\text{C2})$$

for the measurement directions on Alice's subsystem, as well as

$$\mathbf{s} = \begin{pmatrix} \cos \theta \cos(\gamma + \delta) \\ \sin \theta \cos(\gamma + \delta) \\ \sin(\gamma + \delta) \end{pmatrix} \quad (\text{C3})$$

and

$$\mathbf{t} = \begin{pmatrix} \cos \theta \cos(\gamma - \delta) \\ \sin \theta \cos(\gamma - \delta) \\ \sin(\gamma - \delta) \end{pmatrix} \quad (\text{C4})$$

for the directions on Bob's subsystem. Here, $\gamma \in [0, 2\pi)$ is a free parameter, while

$$\delta = \text{arccot} \sqrt{\frac{\mathcal{C}^2 \cos^2 \gamma + \sin^2 \gamma}{\mathcal{C}^2 \sin^2 \gamma + \cos^2 \gamma}} \quad (\text{C5})$$

also depends on γ .

1. Relative coordinates between the measurements $\mathbf{Q}$ and $\mathbf{R}$

We are now in the position to calculate the angle difference of the measurements on Alice's subsystem.

According to the definition in Appendix A, the angle difference $\Delta_{QR} = \vartheta_Q - \vartheta_R$ is defined by the polar angles ϑ_Q and ϑ_R of the measurement directions in spherical coordinates. In Ref. [13], we have already shown that these angles are given by

$$\vartheta_Q = \arctan \left(-\frac{1}{\mathcal{C}} \cot \gamma \right) \quad (\text{C6})$$

and

$$\vartheta_T = \arctan \left(\frac{1}{\mathcal{C}} \tan \gamma \right). \quad (\text{C7})$$

Thus, we find

$$\Delta_{QR} = -\arctan \left(\frac{1}{\mathcal{C}} \cot \gamma \right) - \arctan \left(\frac{1}{\mathcal{C}} \tan \gamma \right) \quad (\text{C8})$$

for the angle difference, where we made use of the symmetry $\arctan(-x) = -\arctan x$.

With help of the relations

$$\arctan x + \arctan y = \arctan \left(\frac{x + y}{1 - xy} \right) \quad (\text{C9})$$

and

$$\cos(\arctan x) = \frac{1}{\sqrt{1 + x^2}}, \quad (\text{C10})$$

we furthermore find

$$\cos \Delta_{QR} = \sqrt{1 + \frac{\mathcal{C}^2}{(1 - \mathcal{C}^2)^2} (\cot \gamma + \tan \gamma)^2}^{-1}. \quad (\text{C11})$$

We now calculate the γ -dependent part

$$(\cot \gamma + \tan \gamma)^2 = \cot^2 \gamma + \tan^2 \gamma + 2 \cot \gamma \tan \gamma. \quad (\text{C12})$$

From the trigonometric relations

$$\cot \gamma \tan \gamma = 1 \quad (\text{C13})$$

and

$$\cot^2 \gamma + 1 = \frac{1}{\sin^2 \gamma}, \quad (\text{C14})$$

as well as

$$\tan^2 \gamma + 1 = \frac{1}{\cos^2 \gamma} \quad (\text{C15})$$

and

$$\frac{1}{\sin^2 \gamma} + \frac{1}{\cos^2 \gamma} = \frac{1}{\sin^2 \gamma \cos^2 \gamma}, \quad (\text{C16})$$

we finally arrive at

$$(\cot \gamma + \tan \gamma)^2 = \frac{1}{\sin^2 \gamma \cos^2 \gamma}. \quad (\text{C17})$$

When we insert this result back into Eq. (C11), we obtain

$$\cos \Delta_{QR} = \frac{(1 - C^2) \sin \gamma \cos \gamma}{\sqrt{C^2 + (1 - C^2)^2 \sin^2 \gamma \cos^2 \gamma}}. \quad (\text{C18})$$

2. Relative coordinates between the measurements T and S

Analogously to the previous subsection, we calculate the relation for the angle difference between the measurement directions for Bob's subsystem. We recall from Appendix A the angle difference $\Delta_{TS} = \vartheta_T - \vartheta_S$. Moreover, according to Eqs. (C3) and (C4), $\vartheta_T = \gamma - \delta$ and $\vartheta_S = \gamma + \delta$, and thus we find

$$\Delta_{TS} = -2\delta. \quad (\text{C19})$$

With help of the relation

$$\cos(2 \operatorname{arccot} y) = \frac{y^2 - 1}{y^2 + 1}, \quad (\text{C20})$$

and with $y^2 = a/b$, we obtain

$$\cos(2 \operatorname{arccot} y) = \frac{a - b}{a + b}. \quad (\text{C21})$$

When we combine this result with our relation for the angle δ , Eq. (C5), we find

$$\cos \Delta_{TS} = \frac{C^2 \cos^2 \gamma + \sin^2 \gamma - C^2 \sin^2 \gamma - \cos^2 \gamma}{C^2 \cos^2 \gamma + \sin^2 \gamma + C^2 \sin^2 \gamma + \cos^2 \gamma} \quad (\text{C22})$$

or

$$\cos \Delta_{TS} = \frac{1 - C^2}{1 + C^2} (\sin^2 \gamma - \cos^2 \gamma), \quad (\text{C23})$$

where in the denominator we again made use of the identity $\cos^2 \gamma + \sin^2 \gamma \equiv 1$.

3. Expectation value of R and S

Finally, we derive the expectation value

$$\langle \hat{R} \otimes \hat{S} \rangle = \mathbf{r}^T K \mathbf{s} \quad (\text{C24})$$

for a joint measurement of $\hat{R}$ and $\hat{S}$. Here, the diagonal matrix

$$K = -\operatorname{diag}(C, C, 1) \quad (\text{C25})$$

is the correlation matrix for the state with concurrence C . When we insert this relation, together with our relations for the measurement directions $\mathbf{r}$ and $\mathbf{s}$, Eqs. (C2) and (C3), into the expectation value, Eq. (C26), we immediately find

$$\langle \hat{R} \otimes \hat{S} \rangle = \frac{C^2 \cos \gamma \cos(\gamma + \delta) + \sin \gamma \sin(\gamma + \delta)}{\sqrt{C^2 \cos^2 \gamma + \sin^2 \gamma}}, \quad (\text{C26})$$

where we made use of the relation $\cos^2 \theta + \sin^2 \theta = 1$.

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