Average correlation as an indicator for nonclassicality

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Bell inequalities are an essential part of quantum information theory. Based on these fundamental inequalities, we propose a different indicator for nonclassicality in the Bell sense: average correlation. We derive a general expression for average correlation and calculate its value for pure states and Werner states. From there we show how two inequalities emerge which serve as necessary and sufficient conditions for nonclassicality. They are simple to evaluate and can even be used to classify all bipartite qubit states.

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I. INTRODUCTION

The study of nonclassical quantum states has had an enormous twofold impact. First, it has completely changed our concept of physical reality [1–3], and second, nowadays possibly even more important, it has led to a new era of quantum technology [4]. Both revolutions have their roots in two fundamental features of quantum states: superposition and entanglement. Already for a single system, e.g., a quantized mode of the electromagnetic field, a suited superposition state will show nonclassical effects like squeezing [5]. One step further, one finds nonlocality, which results from the nonclassical correlations between at least two entangled systems. Both effects have paved the way to new technological applications [4].

Consequently, an important question has always been whether we can measure nonclassicality in the underlying quantum states. In the literature, one can find various measures of nonclassicality, which are discussed more in detail in Refs. [6,7]. These measures are mostly related to the structure of quantum states in Hilbert space. However, nonclassicality rather means that we have no classical model to describe experimental data observed for physical systems described by a specific quantum state. Hence, to quantify nonclassicality one has to take into account certain properties of a physical observable and its statistics for a given state. Regarding entangled systems, the well-known Bell inequalities are probably the best example for this combination. John Bell introduced [8] the Bell inequality as a way to tell how quantum physics provides certain predictions on such systems that cannot be explained by a locally causal model. Moreover, these predictions can be tested experimentally [2].

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The inequality is based on correlation functions of dichotomic observables measured by two distant observers A and B. The correlation function

$$E(\mathbf{a},\mathbf{b}) \equiv \mathrm{tr}(\hat{\rho}\,\mathbf{a}\cdot\hat{\boldsymbol{\sigma}}_A \otimes \mathbf{b}\cdot\hat{\boldsymbol{\sigma}}_B) \tag{1}$$

represents the quantum counterpart for a system in a state $\hat{\rho}$. Unit vectors $\mathbf{a}$ and $\mathbf{b}$ determine the measurement axis of each observer with Pauli spin vectors $\hat{\boldsymbol{\sigma}}_A = (\hat{\sigma}_{1A}, \hat{\sigma}_{2A}, \hat{\sigma}_{3A})$ and $\hat{\boldsymbol{\sigma}}_B = (\hat{\sigma}_{1B}, \hat{\sigma}_{2B}, \hat{\sigma}_{3B})$.

There are several ways of constructing a Bell inequality, but a well established form uses the sum [2,9]

$$\begin{aligned} S(\mathbf{a},\mathbf{a}';\mathbf{b},\mathbf{b}') \equiv |&E(\mathbf{a},\mathbf{b}) + E(\mathbf{a}',\mathbf{b}) \\ &+ E(\mathbf{a},\mathbf{b}') - E(\mathbf{a}',\mathbf{b}')| \end{aligned} \tag{2}$$

which is based on four correlation functions, Eq. (1), and four measurement directions: $(\mathbf{a},\mathbf{a}')$ for observer A and $(\mathbf{b},\mathbf{b}')$ for observer B.

Originally, Bell sums had the aim to verify [10–16] that quantum nature is indeed nonlocal since the sum, Eq. (2), reaches values

$$2 < S \leqslant 2\sqrt{2}$$

depending on the measurement directions and the underlying quantum state. This regime cannot be explained by a locally causal theory.

However, in the sense just mentioned, Bell sums can also be used to quantify nonclassicality [17–20], since they build upon experimentally accessible correlations. The maximum of a Bell sum often serves as a nonclassicality measure, meaning the higher the maximum, the more nonclassical a state $\hat{\rho}$ is expected to be [20].

Operationally, it is no simple task to detect this maximum. Even for a nonclassical state, many of the aforementioned measurement directions in Eq. (2) will not lead to a Bell sum $S > 2$. The aim of our work is to introduce and analyze an operationally simpler correlation function, which still indicates nonclassicality in the Bell sense.

The paper is organized as follows: In Sec. II we define average correlation and give a general expression and its fundamental boundaries. Then in Sec. III we compute average correlation for pure states and Werner states and describe how average correlation can be used to indicate nonclassicality. Finally, in Sec. IV we discuss how generic mixed states fit into the picture and in Sec. V we conclude and give a brief outlook. In Appendix A, we derive general expressions for average correlation. In Appendix B we show the monotony of average correlation in different parameters. Moreover, we prove the fundamental boundaries for average correlation. Eventually, in Appendix C we specify average correlation for different classes of states used throughout the main body of our article.

II. AVERAGE CORRELATION AND ITS FUNDAMENTAL BOUNDARIES

The value of a Bell sum, Eq. (2), is our central criterion to classify nonclassicality of a state $\hat{\rho}$. We define a state to be nonclassical if it leads to a sum $S > 2$ in any configuration. However, we no longer evaluate a Bell sum, Eq. (2), but use average correlation

$$\Sigma \equiv \frac{1}{(4\pi)^2} \int d\Omega_{\mathbf{a}} \int d\Omega_{\mathbf{b}} |E(\mathbf{a}, \mathbf{b})|, \tag{3}$$

which is based on the modulus of the bipartite correlation function, Eq. (1), averaged over all measurement directions **a** and **b**.

We will show that average correlation indicates nonclassicality. As opposed to evaluating Bell inequalities, Σ has the operational advantage that averaging correlations does not require good control of measurement directions. When Bell sums are measured, one needs to fix two measurement directions for each subsystem. On top of that, the detection of a Bell sum requires precise measurements, since any value of the Bell sum in the range $S > 2$ indicates nonclassicality. Average correlation Σ on the other hand can be determined by simply measuring several correlations at random and averaging their absolute values. Therefore, average correlation is a quantity independent of any shared reference frame. We emphasize here that this concept of randomized measurements has been applied earlier to detect nonclassical features of quantum systems in other quantities [17–19,21–26].

The aforementioned simplicity is also in contrast to other nonclassicality measures, as they typically involve a minimization or maximization over all measurements, such as for quantum discord [27] or symmetric discord [28]. While this can be simple to calculate for certain classes of states, it can prove to be harder in general and experimentally not as straightforward. Other measures that are simpler to calculate often suffer from a lack of generality, such as measurement-induced disturbance [29].

In order to study the predictions that one can make with certain values of Σ, Eq. (3), we rewrite the correlation function, Eq. (1), in the form

$$E(\mathbf{a}, \mathbf{b}) = \mathbf{a}^T K \mathbf{b} \tag{4}$$

using the correlation matrix K with elements

$$K_{ij} = \mathrm{tr}(\hat{\rho}\, \hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}), \tag{5}$$

which contains all the information necessary for our purpose about the state $\hat{\rho}$. Furthermore, for any correlation matrix K exists [30] a decomposition with nonnegative singular values

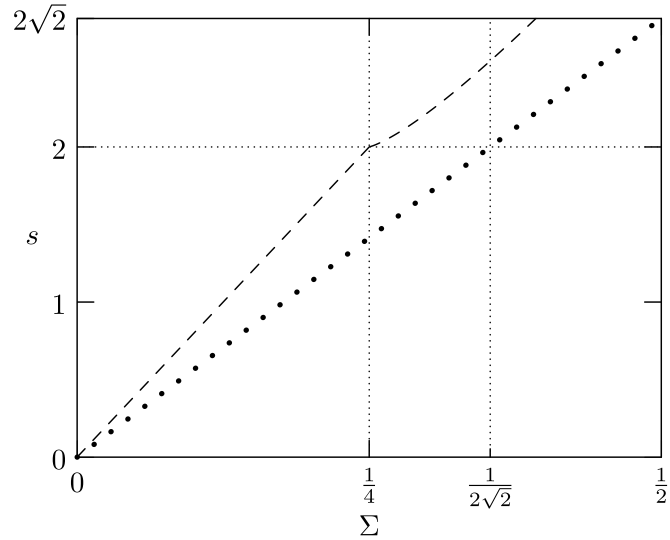

FIG. 1. Bell parameter s as a function of average correlation Σ for two fundamental boundaries: The upper boundary (dashed line) represents the function $s = s(\Sigma_{\min})$ and the lower boundary (dotted line) depicts the curve $s = s(\Sigma_{\max})$. All bipartite qubit states are located between these two boundaries. It can be seen that both boundaries are strictly monotonically increasing in Σ and reach the nonclassical regime $s > 2$ for two critical values $\Sigma = 1/4$ and $\Sigma = 1/2\sqrt{2}$.

$\alpha \geqslant \beta \geqslant \gamma \geqslant 0$; see Appendix A. We also recall [30] that for any state the maximum of the Bell sum, Eq. (2), is given by

$$s \equiv 2\sqrt{\alpha^2 + \beta^2} \tag{6}$$

and hence it is useful to introduce the so-defined Bell parameter s, Eq. (6), in order to quantify the possibility of reaching the nonclassical regime $s > 2$. Based on the state-dependent parameters α, s, and γ, we show in Appendix A that average correlation, Eq. (3), has the general form

$$\begin{aligned}\Sigma &= \Sigma(\alpha, s, \gamma)\\ &= \frac{\alpha}{8\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \sqrt{f(\phi)\sin^2\theta + \cos^2\theta}\end{aligned} \tag{7}$$

with a function

$$f(\phi) \equiv \frac{s^2 - 4\alpha^2}{4\alpha^2} \sin^2\phi + \frac{\gamma^2}{\alpha^2} \cos^2\phi. \tag{8}$$

This general expression turns out to be particularly important since we can apply it to prove fundamental boundaries of Σ as a function of the Bell parameter s. Indeed, maximizing and minimizing $\Sigma(\alpha, s, \gamma)$ over α and γ give us a minimal value $\Sigma_{\min}(s)$ and a maximal value $\Sigma_{\max}(s)$, respectively; see Appendix B. All two-qubit states with a certain Bell parameter s must lie in between these boundaries.

Figure 1 depicts these boundaries and clearly shows their monotony. Note that we consider average correlation as our operational quantity, which allows us to infer nonclassicality via the Bell parameter s. Hence, we plot these boundaries as functions $s = s(\Sigma_{\min})$ and $s = s(\Sigma_{\max})$. It can be seen that the upper and lower boundaries eventually reach the nonclassical regime $s > 2$ for corresponding values of $\Sigma = 1/4$ and

$\Sigma = 1/2\sqrt{2}$, respectively. Hence, based on these fundamental boundaries we can conjecture that $\Sigma > 1/4$ represents a necessary condition for the nonclassicality of an unknown two-qubit state, whereas $\Sigma > 1/2\sqrt{2}$ is a sufficient condition.

However, so far, our discussion has solely focused on the mathematical structure of Σ, Eq. (7). In the following section, we will put average correlation to the test by applying the general expression, Eq. (7), to explicitly determine average correlation for two well-known classes of states: pure states and Werner states. Based on these states, we will answer the question whether the two theoretical boundaries shown in Fig. 1 can actually be reached by physical states and whether the inequalities $\Sigma > 1/4$ and $\Sigma > 1/2\sqrt{2}$ translate into physical criteria.

III. INDICATING NONCLASSICALITY

Pure states as well as Werner states are well known to play a significant role in the discussion of nonclassical Bell sums [2]. Hence, it is to be expected that they behave similarly in a discussion of their respective average correlation.

A. Pure states

We start our analysis with bipartite pure states $|\Psi\rangle$ since any degree of entanglement [31] can lead to a Bell sum $S > 2$. We express pure states in Schmidt decomposition,

$$|\Psi\rangle = c|0\rangle_A|1\rangle_B - \sqrt{1-c^2}|1\rangle_A|0\rangle_B \qquad (9)$$

with a superposition parameter $c \in [0, 1/\sqrt{2}]$ and the computational basis states $|0\rangle_A, |1\rangle_A$ for system A and $|0\rangle_B, |1\rangle_B$ for system B. For this particular set of states the Bell parameter, Eq. (6), reads

$$s = 2\sqrt{1 + 4c^2(1-c^2)} \qquad (10)$$

and we arrive at the average correlation, Eq. (7),

$$\Sigma_{\mathrm{p}}(s) = \frac{1}{4}\left[1 + \frac{s^2-4}{2\sqrt{8-s^2}}\mathrm{Arsinh}\left(\sqrt{\frac{8-s^2}{s^2-4}}\right)\right]. \qquad (11)$$

Both results are derived in Appendix C. We emphasize that average correlation for pure states, Eq. (11), is a monotonically increasing function in the Bell parameter s. Product states, i.e., $c = 0$ or $s = 2$, lead to the lowest value $\Sigma = 1/4$. For values $\Sigma > 1/4$ we need entanglement, i.e., $c \in (0, 1/\sqrt{2}]$ up to $\Sigma = 1/2$ for maximally entangled states, i.e., $c = 1/\sqrt{2}$ or $s = 2\sqrt{2}$. Hence, we conclude that at least for pure states the value of average correlation allows us to infer nonclassicality. This becomes even clearer when we use Eq. (11) to plot the Bell parameter s as a function of average correlation Σ_{p}; see Fig. 2. As expected, we obtain a curve in between the boundaries derived in the previous section.

B. Werner states

Next, we discuss Werner states [32]

$$\hat{\rho}_{\mathrm{W}} \equiv \lambda|\Psi^{(-)}\rangle\langle\Psi^{(-)}| + \frac{1-\lambda}{4}\hat{\mathbb{1}}, \qquad (12)$$

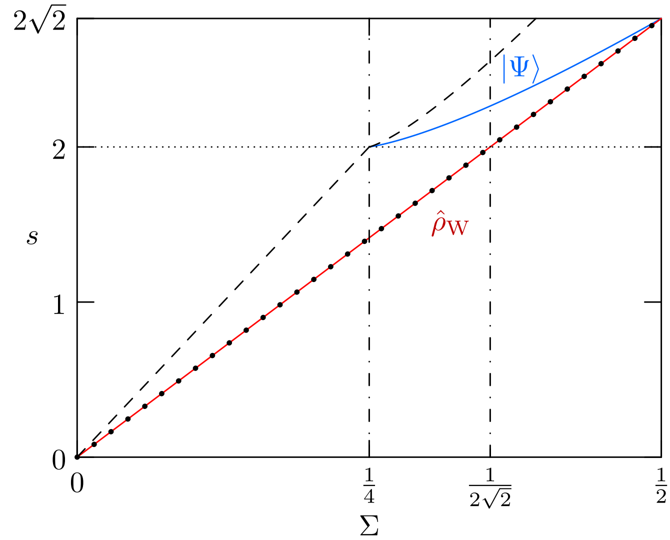

FIG. 2. Bell parameter s as a function of average correlation Σ for pure states $|\Psi\rangle$ (solid blue line) and Werner states $\hat{\rho}_{\mathrm{W}}$ (solid red line) together with the upper (dashed line) and lower boundaries (dotted line) already shown in Fig. 1. The curves of both classes of states are given analytically by Eqs. (11) and (15). Werner states lead exactly to the linear behavior of the lower boundary, and the corresponding average correlation Σ as well as the Bell parameter s span the full interval of possible values. Moreover, Werner states need a considerable amount of average correlation $\Sigma > 1/2\sqrt{2}$ before they become nonclassical, i.e., $s > 2$. As expected, pure states are quite different. Obviously, they mark the true upper boundary in the nonclassical region $s > 2$. Their average correlation never falls below $\Sigma = 1/4$, which holds for product states. Pure states, which are entangled, will be clearly nonclassical with an average correlation $\Sigma > 1/4$. Hence, the critical values $\Sigma = 1/4$ and $\Sigma = 1/2\sqrt{2}$ now obtain a physical meaning since they can be reached by physical states: They separate the purely classical regime, i.e., $\Sigma \leqslant 1/4$, from the purely nonclassical counterpart, i.e., $\Sigma > 1/2\sqrt{2}$.

which combine the completely mixed state $\hat{\mathbb{1}}/4$ with a maximally entangled Bell state

$$|\Psi^{(-)}\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A|1\rangle_B - |1\rangle_A|0\rangle_B), \qquad (13)$$

weighted by the visibility $\lambda \in [0, 1]$.

Werner states are particularly interesting from the point of view of nonclassicality. They result in a classical Bell sum $S \leqslant 2$ for visibilities $\lambda \in [0, 1/\sqrt{2}]$ even though the corresponding density operator, Eq. (12), is not separable [32] for visibilities $\lambda \in (1/3, 1]$. Thus, in the interval $\lambda \in (1/3, 1/\sqrt{2}]$ Werner states are not separable but behave classically under Bell measurements. A nonclassical Bell sum $S > 2$ can only be found in the range $\lambda \in (1/\sqrt{2}, 1]$. In fact, for Werner states the Bell parameter, Eq. (6), reads

$$s = 2\sqrt{2}\lambda \qquad (14)$$

and average correlation is given by

$$\Sigma_{\mathrm{W}}(s) = \frac{s}{4\sqrt{2}}, \qquad (15)$$

as again shown in Appendix C. As opposed to pure states, average correlation of Werner states can take on all values in the interval $\Sigma \in [0, 1/2]$. We again show the Bell parameter s as a function of Σ_W; see Fig. 2. Remarkably, Werner states are found precisely at the lower boundary discussed in the previous section.

The fact that the critical points $\Sigma = 1/4$ and $\Sigma = 1/2\sqrt{2}$ at $s = 2$ are reached by pure states and Werner states now gives them a clear physical significance. In accordance with our previous conjecture, we can now clearly assert the following: For $\Sigma \leqslant 1/4$ we find only classical states, for $\Sigma > 1/2\sqrt{2}$ only nonclassical states, and for $1/4 < \Sigma \leqslant 1/2\sqrt{2}$ both classical and nonclassical states exist. In this way, average correlation Σ can be used as an indicator for nonclassicality as we have both a necessary, $\Sigma > 1/4$, and a sufficient condition, $\Sigma > 1/2\sqrt{2}$, for nonclassicality.

As Werner states become nonclassical for the largest possible value of $\Sigma = 1/2\sqrt{2}$, while pure states immediately become nonclassical for the lowest possible value of $\Sigma = 1/4$, one may consider them two extreme cases. In other words, in the nonclassical regime, i.e., for $s > 2$, we expect that all states will be found in between pure states and Werner states. In the next section, we will study the behavior of arbitrary mixed states in order to elaborate on this point and to complete the picture.

IV. A MAP OF ALL STATES

The results so far, shown in Fig. 2, have given us essential insight into novel criteria regarding nonclassicality. As a last step, we would like to gain a deeper understanding of a complete Σ-s mapping for all two-qubit states. In particular, we have not yet understood whether the upper boundary in the classical regime, i.e., $\Sigma \leqslant 1/4$ will be reached by a physical state. Hence, we add a discussion for arbitrary mixed states to see how they complement our findings so far.

In order to do so, we have numerically computed average correlation, Eq. (7), for a random ensemble of mixed states [33]. This evaluation is depicted in Fig. 3, in which we again represent the Bell parameter s as a function of average correlation Σ. Moreover, the analytical curves for Werner states and pure states are also shown as in Fig. 2.

From the numerics and the previous discussion, we now recognize, that two-qubit states completely fill the Σ-s map shown in Fig. 3. In the purely classical regime, i.e., $\Sigma \leqslant 1/4$, the upper boundary will be reached by physical states. In fact this class of states is given by separable mixed states of the form [34]

$$\hat{\rho}_\xi = \frac{1+\xi}{2}|1\rangle\langle 1|_A \otimes |0\rangle\langle 0|_B + \frac{1-\xi}{2}|0\rangle\langle 0|_A \otimes |0\rangle\langle 0|_B \tag{16}$$

for $0 \leqslant \xi \leqslant 1$. This class of states is also discussed in Ref. [35], where it also marks a boundary in a mapping of two-qubit states. The corresponding average correlation reads

$$\Sigma_\xi = \frac{\xi}{4} = \frac{s}{8}, \tag{17}$$

which is also shown in Appendix C.

Therefore, Fig. 3 can be considered a complete map of all states and their location in the three previously discussed domains. For $\Sigma \leqslant 1/4$ we only find classical states, colored in yellow, while for $\Sigma > 1/2\sqrt{2}$ we only find nonclassical states, colored in blue. For $1/4 < \Sigma \leqslant 1/2\sqrt{2}$, however, we find states that can be both classical and nonclassical, colored in green.

Finally, we recognize that pure states are the true upper boundary in the nonclassical regime in the Σ-s map.

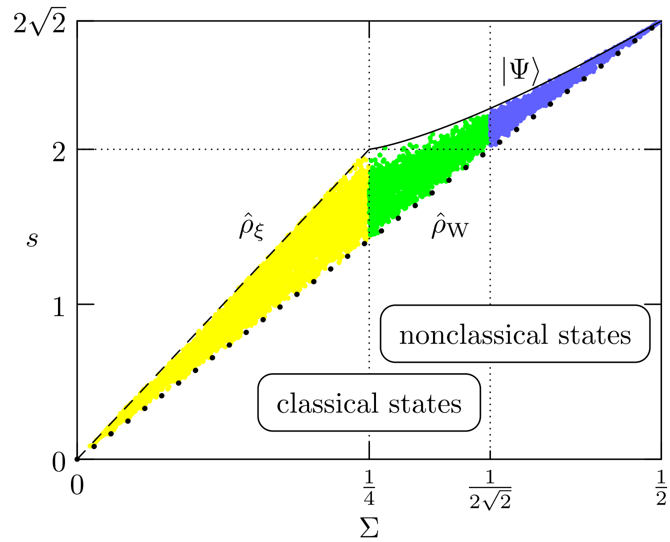

FIG. 3. Bell parameter s as a function of average correlation Σ for all bipartite qubit states. The analytic results for the upper (dashed line) and lower boundaries (dotted line) as well as for pure states $|\Psi\rangle$ (solid line) have been transferred from Fig. 2. Werner states $\hat{\rho}_W$ and ξ states $\hat{\rho}_\xi$ are located at the lower boundary and the upper boundary between $s = 0$ and $s = 2$, respectively. In between, we find the colored points for arbitrary mixed states, which have been generated numerically. Average correlations $\Sigma > 1/2\sqrt{2}$ necessarily indicate nonclassical states. Moreover, these states are wedged between Werner states, which are the least nonclassical, and pure states. Average correlations in the interval $1/4 < \Sigma \leqslant 1/2\sqrt{2}$ are still embedded in this wedge, but the corresponding states can be classical or nonclassical. Finally, we reach the classical wedge for values $\Sigma \leqslant 1/4$. Its lower boundary is still given by Werner states, but the upper boundary (dashed line) is a different class of mixed states that, just like Werner states, leads to a linear behavior.

V. CONCLUSIONS AND OUTLOOK

In summary, we have shown that average correlation Σ leads to two inequalities of nonclassicality with $\Sigma \leqslant 1/4$ corresponding to only classical states and $\Sigma > 1/2\sqrt{2}$ corresponding to only nonclassical states. Moreover, Σ is easy to calculate via the presented general expression and, due to its operational definition, it is a measurable quantity. For all of these reasons, Σ can be considered a good indicator for nonclassicality. We emphasize that we have defined nonclassicality in the Bell sense. However, there are numerous ways of defining nonclassicality [36].

There are still open problems that remain to be solved. For one, it is an interesting question what physical constraints lead to the upper boundary given by pure entangled states. Second, other indicators and measures for nonclassicality have been proposed. Like average correlation discussed here, they are based on random measurements [17–19,25]. Comparing average correlation to such measures could yield further interesting insights. Lastly, we have taken note of the work of Morelli *et al.* [35]. In their work, the authors map two-qubit states based on a norm of the correlation matrix and the lengths of the two local Bloch vectors of both systems. The boundaries discussed in our work are also boundaries in their mapping. Finding out what is the deeper physical reason behind this similarity is a fascinating problem and could give us an even better understanding of our mapping of average correlation.

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APPENDIX A: GENERAL EXPRESSION FOR AVERAGE CORRELATION

In this appendix, we derive a general expression for average correlation Σ, Eq. (3), as a function of singular values which define the correlation matrix, Eq. (5).

We recall that the correlation function, Eq. (1), can be rewritten in the form

$$E(\mathbf{a}, \mathbf{b}) = \mathbf{a}^T K \mathbf{b} = \sum_{i,j} a_i K_{ij} b_j, \quad \text{(A1)}$$

where we defined [30] the correlation matrix K with elements

$$K_{ij} = \mathrm{tr}(\hat{\rho}\, \hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}) \quad \text{(A2)}$$

for an arbitrary state $\hat{\rho}$. For this correlation matrix K, there exists a singular value decomposition [30]

$$K = U \kappa V^T \quad \text{(A3)}$$

with two orthogonal matrices U and V and the diagonal matrix

$$\kappa = \mathrm{diag}(\alpha, \beta, \gamma), \quad \text{(A4)}$$

which can be chosen in a way such that the singular values $\alpha \geqslant \beta \geqslant \gamma \geqslant 0$ are nonnegative. Since U and V are orthogonal, they simply rotate the vectors $\mathbf{a}$ and $\mathbf{b}$ but leave their norms invariant. Thus, the vectors

$$\tilde{\mathbf{a}} = U^T \mathbf{a},\ \tilde{\mathbf{b}} = V^T \mathbf{b} \quad \text{(A5)}$$

are unit vectors, too. Hence, we can rewrite average correlation, Eq. (3), as

$$\Sigma = \frac{1}{16\pi^2} \int d\Omega_{\mathbf{a}} \int d\Omega_{\mathbf{b}} |(\tilde{\mathbf{a}})^T \tilde{\mathbf{b}}_\kappa|, \quad \text{(A6)}$$

where the integrand is given by the modulus of a scalar product between the unit vector $\tilde{\mathbf{a}}$ and the vector

$$\tilde{\mathbf{b}}_\kappa = \kappa \tilde{\mathbf{b}}. \quad \text{(A7)}$$

Furthermore, the scalar product can be expressed by the length of the vectors and the angle θ_{AB} between them, leading to

$$\Sigma = \frac{1}{16\pi^2} \int d\Omega_{\mathbf{a}} \int d\Omega_{\mathbf{b}} |\tilde{\mathbf{b}}_\kappa| |\cos\theta_{AB}|. \quad \text{(A8)}$$

We are now in the position to integrate over all measurement settings of the vector $\tilde{\mathbf{a}}$. In order to simplify this integration, we choose spherical coordinates and set the z-axis of the coordinate system to align with the vector $\tilde{\mathbf{b}}_\kappa$. As a consequence, the angle θ_{AB} corresponds to the polar angle, while the integrand is independent of the azimuthal angle. The integration over $d\Omega_{\mathbf{a}}$ is then straightforward, and we obtain

$$\Sigma = \frac{1}{8\pi} \int d\Omega_{\mathbf{b}} |\tilde{\mathbf{b}}_\kappa|. \quad \text{(A9)}$$

We solve the remaining integral by choosing spherical coordinates so that we can write

$$\tilde{\mathbf{b}}_\kappa = (\gamma \cos\phi \sin\theta, \beta \sin\phi \sin\theta, \alpha \cos\theta)^T, \quad \text{(A10)}$$

giving us

$$\Sigma = \frac{\alpha}{8\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \sqrt{f(\phi) \sin^2\theta + \cos^2\theta}, \quad \text{(A11)}$$

where we have defined the function

$$f(\phi) \equiv \left(\frac{\beta}{\alpha}\right)^2 \sin^2\phi + \left(\frac{\gamma}{\alpha}\right)^2 \cos^2\phi. \quad \text{(A12)}$$

By substituting $u = \cos\theta$ and rearranging terms, we find the integral

$$\Sigma = \frac{\alpha}{8\pi} \int_0^{2\pi} d\phi \sqrt{f(\phi)} \int_{-1}^{1} du \sqrt{1 + \frac{1 - f(\phi)}{f(\phi)} u^2}, \quad \text{(A13)}$$

which can be further reduced to the general expression

$$\Sigma = \frac{\alpha}{4}\left[1 + \frac{1}{2\pi}\int_0^{2\pi} d\phi \frac{f(\phi)}{\sqrt{1 - f(\phi)}} \mathrm{Arsinh}\left(\sqrt{\frac{1 - f(\phi)}{f(\phi)}}\right)\right], \quad \text{(A14)}$$

which now involves only one integration. Furthermore, with the help of Refs. [37,38] we recognize that average correlation is proportional to the surface area of an ellipsoid with semiaxes $\sqrt{(\alpha\beta)/\gamma}$, $\sqrt{(\alpha\gamma)/\beta}$, and $\sqrt{(\beta\gamma)/\alpha}$, which enables us to write

$$\Sigma = \frac{\gamma}{4}\left(\frac{\beta}{\alpha} + \frac{\sqrt{\alpha^2 - \gamma^2}}{\gamma} E(\varphi, k) + \frac{\gamma}{\sqrt{\alpha^2 - \gamma^2}} F(\varphi, k)\right), \quad \text{(A15)}$$

with arguments

$$\varphi \equiv \arcsin\left(\frac{\sqrt{\alpha^2 - \gamma^2}}{\alpha}\right), \quad k \equiv \sqrt{\frac{\alpha^2 - \beta^2}{\alpha^2 - \gamma^2}}. \quad \text{(A16)}$$

in terms of the incomplete elliptic integrals F and E of the first and second kind, respectively. We will apply this representation in Appendix B to prove fundamental boundaries of average correlation.

APPENDIX B: BOUNDARIES FOR AVERAGE CORRELATION

In this appendix, we derive the lower and upper boundary, as discussed in Fig. 1. In order to do so, we first show that $\Sigma(\alpha, s, \gamma)$, Eq. (A14), increases monotonically in the smallest singular value γ of the correlation matrix, if the largest singular value α and the Bell parameter s are fixed.

1. Monotony of average correlation

In order to prove monotony in γ, we remark that γ only enters in Σ via the function f, which is part of the integrand; see Eq. (A14). Therefore, we first show that the integrand is monotonically increasing in f. For this purpose, we consider the function

$$g(x) \equiv \frac{x}{\sqrt{1-x}}\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) \tag{B1}$$

and argue that it is a monotonically increasing function on the interval $x \in (0, 1)$. Hence, the derivative

$$\frac{dg}{dx} = \frac{2-x}{2\sqrt{1-x}^3}\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) - \frac{1}{2(1-x)} \tag{B2}$$

has to be positive for all values of $x \in (0, 1)$, that is

$$\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) > \frac{\sqrt{1-x}}{2-x}. \tag{B3}$$

For the left-hand side of Eq. (B3) we can write

$$\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) \geqslant \mathrm{Arsinh}(\sqrt{1-x}) \geqslant \frac{\sqrt{1-x}}{6}(5+x), \tag{B4}$$

where we have used the Taylor expansion of the inverse hyperbolic sine in the second step. The obvious inequality

$$\frac{1}{6}(5+x) > \frac{1}{2-x} \tag{B5}$$

is satisfied on the interval $x \in (0, 1)$ which finally proves Eq. (B3). Thus, the function g, Eq. (B1), is monotonically increasing.

Next, we note that for every value of the azimuthal angle ϕ, the function

$$f(\phi) \equiv \frac{s^2 - 4\alpha^2}{4\alpha^2}\sin^2\phi + \frac{\gamma^2}{\alpha^2}\cos^2\phi \tag{B6}$$

is also monotonically increasing in the singular value γ, for fixed parameters s and α. Consequently, the composite function $g(f(\phi))$ and with it average correlation Σ are, too.

2. Maximum of average correlation

We are now in a position to derive the maximum of average correlation $\Sigma = \Sigma(\alpha, s, \gamma)$, Eq. (7), with respect to the singular values γ and α resulting in $\Sigma_{\max} = \Sigma_{\max}(s)$ which is strictly monotonically increasing in the Bell parameter s.

As we have shown above, average correlation $\Sigma(\alpha, s, \gamma)$ is monotonically increasing in γ and thus becomes maximal for a maximal value of $\gamma = \gamma_{\max} = \beta = \sqrt{s^2/4 - \alpha^2}$, which reduces $f(\phi)$, Eq. (A12), to

$$f(\phi) = \frac{s^2 - 4\alpha^2}{4\alpha^2} \tag{B7}$$

and allows us to write

$$\alpha = \frac{s}{2}\frac{1}{\sqrt{1+f}}. \tag{B8}$$

Using Eq. (A14) we can then express average correlation

$$\Sigma(\alpha, s, \gamma = \gamma_{\max}) = \frac{s}{8}\frac{1}{\sqrt{1+f}}\left[1 + \frac{f}{\sqrt{1-f}}\mathrm{Arsinh}\left(\sqrt{\frac{1-f}{f}}\right)\right] \tag{B9}$$

as a function of s and f. As a next step, we will show that Σ is monotonically increasing in f. For that we consider the function

$$h(x) = \frac{1}{\sqrt{1+x}}\left[1 + \frac{x}{\sqrt{1-x}}\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right)\right] \tag{B10}$$

with its derivative

$$\frac{d}{dx}h(x) = \frac{1}{\sqrt{1-x^2}^3}\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) - \frac{1}{2\sqrt{1+x}^3} - \frac{1}{2\sqrt{(1-x^2)(1-x)}}, \tag{B11}$$

which has to be positive for all $x \in (0, 1)$, that is

$$\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) - \sqrt{1-x} \geqslant 0. \tag{B12}$$

We note that the left-hand side of Eq. (B12) goes to plus infinity for $x \to 0$ and has a zero for $x = 1$. Further, the expression is monotonic since its derivative

$$\frac{d}{dx}\left[\mathrm{Arsinh}\left(\sqrt{\frac{1-x}{x}}\right) - \sqrt{1-x}\right] = -\frac{\sqrt{1-x}}{2x} \tag{B13}$$

is always negative on the considered interval, which proves Eq. (B12). Consequently, the function $h(x)$, Eq. (B10), is monotonically increasing in x. Hence, average correlation, Eq. (B9), is monotonically increasing in f and becomes maximal for the maximal value $f = 1$.

Using Eq. (B9) and the limit

$$\lim_{f\to 1}\frac{1}{\sqrt{1+f}}\left[1 + \frac{f}{\sqrt{1-f}}\mathrm{Arsinh}\left(\sqrt{\frac{1-f}{f}}\right)\right] = \sqrt{2} \tag{B14}$$

the maximum of average correlation then evaluates to

$$\Sigma_{\max}(s) = \frac{s}{4\sqrt{2}}, \tag{B15}$$

which is strictly monotonically increasing in the Bell parameter s.

3. Minimum of average correlation

Next, we derive the minimum of average correlation, that is we minimize $\Sigma = \Sigma(\alpha, s, \gamma)$, Eq. (7), with respect to the singular values γ and α. This results in $\Sigma_{\min} = \Sigma_{\min}(s)$ which is also strictly monotonically increasing in the Bell parameter s.

We first remark that, as shown in Appendix B 1, for fixed values of α and s, $\Sigma = \Sigma(\alpha, s, \gamma)$, Eq. (7), is monotonically increasing in γ and thus becomes minimal for $\gamma = 0$.

Using Eqs. (A15) and (A16) average correlation then reads

$$\Sigma(\alpha, s, \gamma = 0) = \frac{\alpha}{4} E\left(\varphi = \frac{\pi}{2},\ k = \sqrt{2 - \frac{s^2}{4\alpha^2}}\right). \tag{B16}$$

When we recall the definition [38] of the elliptic integral $E = E(\varphi, k)$ we get

$$\Sigma(\alpha, s, \gamma = 0) = \frac{\alpha}{4} \int_0^{\frac{\pi}{2}} dx \sqrt{1 - \left(2 - \frac{s^2}{4\alpha^2}\right)\sin^2 x}. \tag{B17}$$

Next we show that this expression is monotonically decreasing in α for a fixed value of s. For that we must have

$$\frac{d}{d\alpha}\Sigma(\alpha, s, \gamma = 0) = \int_0^{\frac{\pi}{2}} dx \frac{1 - 2\sin^2 x}{4\sqrt{1 - k^2 \sin^2 x}} \leqslant 0. \tag{B18}$$

This condition can be rewritten in the form

$$\int_0^{\pi/4} dx \left(\frac{1 - 2\sin^2 x}{4\sqrt{1 - k^2\sin^2 x}} + \frac{1 - 2\cos^2 x}{4\sqrt{1 - k^2\cos^2 x}}\right) \leqslant 0, \tag{B19}$$

which means for the integrand

$$\frac{1 - 2\sin^2 x}{\sqrt{1 - k^2 \sin^2 x}} \leqslant \frac{2\cos^2 x - 1}{\sqrt{1 - k^2\cos^2 x}} \tag{B20}$$

or

$$1 - k^2 \sin^2 x \geqslant 1 - k^2 \cos^2 x. \tag{B21}$$

This inequality is satisfied for all $x \in [0, \pi/4]$. Thus, for $\gamma = 0$ and any fixed value of s, average correlation is monotonically decreasing in α and therefore becomes minimal for the maximal value $\alpha = 1$ [39].

Furthermore, due to the definition of the Bell parameter

$$s = 2\sqrt{\alpha^2 + \beta^2}, \tag{B22}$$

α is maximally $s/2$, too, so in total we have

$$\min\left(1, \frac{s}{2}\right) \geqslant \alpha. \tag{B23}$$

Hence, in the regime $s \leqslant 2$ we have $\alpha = s/2$, $\beta = \gamma = 0$ and in the regime $s > 2$ we have $\alpha = 1$, $\beta = \sqrt{(s/2)^2 - 1}$, $\gamma = 0$.

With the help of Eqs. (B16) and (B17) we arrive at

$$\Sigma_{\min}(s) = \begin{cases} \frac{s}{8}, & s \leqslant 2, \\ \frac{1}{4}E\left(\varphi = \frac{\pi}{2},\ k = \sqrt{2 - \frac{s^2}{4\alpha^2}}\right), & s > 2, \end{cases} \tag{B24}$$

which is strictly monotonically increasing in s due to the properties of the elliptic integral [38]. In particular, we emphasize the value

$$\Sigma_{\min}(s = 2) = \tfrac{1}{4}, \tag{B25}$$

which is essential in understanding Fig. 1.

APPENDIX C: AVERAGE CORRELATION FOR DIFFERENT CLASSES OF STATES

In this appendix we specify average correlation Σ, Eq. (7), for pure states, Werner states, and ξ states and discuss the corresponding monotony in the Bell parameter s.

1. Pure states

For pure states in Schmidt decomposition,

$$|\Psi\rangle = c|0\rangle_A|1\rangle_B - \sqrt{1 - c^2}|1\rangle_A|0\rangle_B, \tag{C1}$$

with a superposition parameter $c \in [0, 1/\sqrt{2}]$, we find a correlation matrix, Eq. (A2),

$$K = -\mathrm{diag}(2c\sqrt{1 - c^2}, 2c\sqrt{1 - c^2}, 1), \tag{C2}$$

which is diagonal [30] and can be brought into the form

$$K = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = U\kappa V^T, \tag{C3}$$

with singular values $\alpha = 1$ and $\beta = \gamma = 2c\sqrt{1 - c^2}$. Hence, we obtain a Bell parameter, Eq. (6),

$$s \equiv 2\sqrt{1 + 4c^2(1 - c^2)}, \tag{C4}$$

and we specify the function, Eq. (A12),

$$f(\phi) = \beta^2 = \frac{s^2}{4} - 1. \tag{C5}$$

By performing the final integration in Eq. (A14) we arrive at average correlation,

$$\Sigma_{\mathrm{p}}(s) = \frac{1}{4}\left[1 + \frac{s^2 - 4}{2\sqrt{8 - s^2}}\mathrm{Arsinh}\left(\sqrt{\frac{8 - s^2}{s^2 - 4}}\right)\right] \tag{C6}$$

for pure states. We note that this correlation reaches its minimal value $\Sigma_{\mathrm{p}} = 1/4$ for $s = 2$, while for $s = 2\sqrt{2}$ we obtain $\Sigma_{\mathrm{p}} = 1/2$ as its maximal value.

2. Werner states

For Werner states, Eq. (12), the correlation matrix [30] reads $K = -\lambda\hat{\mathbb{1}}$ and leads to three equal singular values $\alpha = \beta = \gamma = \lambda$ and $f = 1$; see Eq. (A12). With the Bell parameter $s = 2\sqrt{2}\lambda$ we find for Werner states

$$\Sigma_{\mathrm{W}}(s) = \frac{s}{4\sqrt{2}} \tag{C7}$$

the same linear average correlation as for the maximum of average correlation; see Appendix B.

3. ξ states

For ξ states, Eq. (16), we get $K = \mathrm{diag}(0, 0, -\xi)$ with singular values $\alpha = \xi$ and $\beta = \gamma = 0$ and thus $f(\phi) = 0$, which are equal to those of the states that make up the upper boundary for $s \leqslant 2$ (see Appendix B) and thus lead to the average correlation

$$\Sigma_\xi(s) = \frac{s}{8} \tag{C8}$$

for ξ states.

[1] A. Einstein, B. Podolsky, and N. Rosen, Can quantum-mechanical description of physical reality be considered complete? Phys. Rev. **47**, 777 (1935).

[2] N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, Bell nonlocality, Rev. Mod. Phys. **86**, 419 (2014).

[3] J. Mehra, *Einstein, Physics and Reality* (World Scientific, Singapore, 1999).

[4] W. P. Schleich, K. S. Ranade, C. Anton, M. Arndt, M. Aspelmeyer, M. Bayer, G. Berg, T. Calarco, H. Fuchs, E. Giacobino *et al.*, Quantum technology: From research to application, Appl. Phys. B **122**, 130 (2016).

[5] L. Davidovich, Sub-Poissonian processes in quantum optics, Rev. Mod. Phys. **68**, 127 (1996).

[6] G. Adesso, T. R. Bromley, and M. Cianciaruso, Measures and applications of quantum correlations, J. Phys. A: Math. Theor. **49**, 473001 (2016).

[7] K. Modi, A. Brodutch, H. Cable, T. Paterek, and V. Vedral, The classical-quantum boundary for correlations: Discord and related measures, Rev. Mod. Phys. **84**, 1655 (2012).

[8] J. S. Bell, On the Einstein Podolsky Rosen paradox, Phys. Phys. Fiz. **1**, 195 (1964).

[9] J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, Proposed Experiment to Test Local Hidden-Variable Theories, Phys. Rev. Lett. **23**, 880 (1969).

[10] S. J. Freedman and J. F. Clauser, Experimental Test of Local Hidden-Variable Theories, Phys. Rev. Lett. **28**, 938 (1972).

[11] E. S. Fry and R. C. Thompson, Experimental Test of Local Hidden-Variable Theories, Phys. Rev. Lett. **37**, 465 (1976).

[12] A. Aspect, J. Dalibard, and G. Roger, Experimental Test of Bell's Inequalities Using Time- Varying Analyzers, Phys. Rev. Lett. **49**, 1804 (1982).

[13] G. Weihs, T. Jennewein, C. Simon, H. Weinfurter, and A. Zeilinger, Violation of Bell's Inequality under Strict Einstein Locality Conditions, Phys. Rev. Lett. **81**, 5039 (1998).

[14] B. Hensen, H. Bernien, A. E. Dréau, A. Reiserer, N. Kalb, M. S. Blok, J. Ruitenberg, R. F. Vermeulen, R. N. Schouten, C. Abellán *et al.*, Loophole-free Bell inequality violation using electron spins separated by 1.3 kilometres, Nature (London) **526**, 682 (2015).

[15] L. K. Shalm, E. Meyer-Scott, B. G. Christensen, P. Bierhorst, M. A. Wayne, M. J. Stevens, T. Gerrits, S. Glancy, D. R. Hamel, M. S. Allman *et al.*, Strong Loophole-Free Test of Local Realism, Phys. Rev. Lett. **115**, 250402 (2015).

[16] M. Giustina, M. A. M. Versteegh, S. Wengerowsky, J. Handsteiner, A. Hochrainer, K. Phelan, F. Steinlechner, J. Kofler, J.-Å. Larsson, C. Abellán, W. Amaya, V. Pruneri, M. W. Mitchell, J. Beyer, T. Gerrits, A. E. Lita, L. K. Shalm, S. W. Nam, T. Scheidl, R. Ursin, B. Wittmann, and A. Zeilinger, Significant-Loophole-Free Test of Bell's Theorem with Entangled Photons, Phys. Rev. Lett. **115**, 250401 (2015).

[17] Y.-C. Liang, N. Harrigan, S. D. Bartlett, and T. Rudolph, Nonclassical Correlations from Randomly Chosen Local Measurements, Phys. Rev. Lett. **104**, 050401 (2010).

[18] J. J. Wallman, Y.-C. Liang, and S. D. Bartlett, Generating nonclassical correlations without fully aligning measurements, Phys. Rev. A **83**, 022110 (2011).

[19] J. J. Wallman and S. D. Bartlett, Observers can always generate nonlocal correlations without aligning measurements by covering all their bases, Phys. Rev. A **85**, 024101 (2012).

[20] J. P. Dahl, H. Mack, A. Wolf, and W. P. Schleich, Entanglement versus negative domains of Wigner functions, Phys. Rev. A **74**, 042323 (2006).

[21] A. Ketterer, N. Wyderka, and O. Gühne, Characterizing Multipartite Entanglement with Moments of Random Correlations, Phys. Rev. Lett. **122**, 120505 (2019).

[22] A. Ketterer, N. Wyderka, and O. Gühne, Entanglement characterization using quantum designs, Quantum **4**, 325 (2020).

[23] S. Imai, N. Wyderka, A. Ketterer, and O. Gühne, Bound Entanglement from Randomized Measurements, Phys. Rev. Lett. **126**, 150501 (2021).

[24] A. Ketterer, S. Imai, N. Wyderka, and O. Gühne, Statistically significant tests of multiparticle quantum correlations based on randomized measurements, Phys. Rev. A **106**, L010402 (2022).

[25] N. Wyderka, A. Ketterer, S. Imai, J. L. Bönsel, D. E. Jones, B. T. Kirby, X.-D. Yu, and O. Gühne, Complete characterization of quantum correlations by randomized measurements, arXiv:2212.07894.

[26] N. Wyderka and A. Ketterer, Probing the geometry of correlation matrices with randomized measurements, arXiv:2211.09610 [PRX Quantum (to be published)].

[27] H. Ollivier and W. H. Zurek, Quantum Discord: A Measure of the Quantumness of Correlations, Phys. Rev. Lett. **88**, 017901 (2001).

[28] D. Girolami, M. Paternostro, and G. Adesso, Faithful nonclassicality indicators and extremal quantum correlations in two-qubit states, J. Phys. A: Math. Theor. **44**, 352002 (2011).

[29] S. Luo, Using measurement-induced disturbance to characterize correlations as classical or quantum, Phys. Rev. A **77**, 022301 (2008).

[30] J. Seiler, T. Strohm, and W. P. Schleich, Geometric interpretation of the Clauser-Horne-Shimony-Holt inequality of nonmaximally entangled states, Phys. Rev. A **104**, 032218 (2021).

[31] N. Gisin, Bell's inequality holds for all non-product states, Phys. Lett. A **154**, 201 (1991).

[32] R. F. Werner, Quantum states with Einstein-Podolsky-Rosen correlations admitting a hidden-variable model, Phys. Rev. A **40**, 4277 (1989).

[33] We generated a random ensemble of 15 126 qubit states and used the singular values of the respective 9070 unique correlation matrices to obtain pairs of Σ and s values.

[34] Note that there are multiple states that constitute the upper boundary and $\hat{\rho}_\xi$, Eq. (16), is only one of them, which we will for the sake of brevity not discuss further in this work.

[35] S. Morelli, C. Eltschka, M. Huber, and J. Siewert, Correlation constraints and the Bloch geometry of two qubits, arXiv:2303.11400.

[36] To better understand the difference between the definition of nonclassicality we used and other definitions we compare average correlation to quantum discord [27] which is widely used in the literature. For Werner states, both quantities yield zero for $s = 0$, and then monotonically increase, reaching their maximal value for $s = 2\sqrt{2}$. Thus, they behave similarly, even though quantum discord does not increase linearly. The difference between average correlation and quantum discord becomes clearer once we take a look at pure states. As before, for pure states, quantum discord monotonically increases from zero to one and thus reaches all possible values [40]. This behavior differs significantly from average correlation, which starts at $\Sigma = 1/4$, while the regime $\Sigma < 1/4$ is not accessible to pure states. Remarkably, for both the completely mixed state and product states, quantum discord yields zero even though their Bell parameters differ by 2. This is what makes average correlation different, which is closer to Bell inequalities in defining nonclassicality.

[37] L. R. Maas, On the surface area of an ellipsoid and related integrals of elliptic integrals, J. Comput. Appl. Math. **51**, 237 (1994).

[38] G. N. Watson, The surface of an ellipsoid, Q. J. Math. **os-6**, 280 (1935).

[39] Since by definition the modulus of the correlation function $|E(\mathbf{a}, \mathbf{b})| = |\mathbf{a}^T K \mathbf{b}| = |(\tilde{\mathbf{a}})^T \mathrm{diag}(\alpha, \beta, \gamma)\tilde{\mathbf{b}}|$ cannot be greater than one, α cannot be greater than one either.

[40] S. Luo, Quantum discord for two-qubit systems, Phys. Rev. A **77**, 042303 (2008).