Average correlation as an indicator for inseparability

Michael E. N. Tschaffon [*] and Johannes Seiler [†]
Institut für Quantenphysik and Center for Integrated Quantum Science and Technology (IQST), Universität Ulm, D-89069 Ulm, Germany

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Inseparability of quantum states is one of the most crucial aspects of quantum physics, as it often provides the key ingredient for obtaining a quantum advantage. Quantifying inseparability is thus an important objective to better understand quantum physics and to improve quantum applications. So far, many measures for inseparability exist, however, most of them are based on abstract mathematical procedures and are not defined operationally which can easily be realized in an experiment. Recently we introduced average correlation [Tschaffon *et al.*, Phys. Rev. Res. **5**, 023063 (2023)] as a reference frame independent indicator for nonclassicality in the Bell sense based on randomized measurements. It is defined as the average absolute value of the two-qubit correlation function and allows one to formulate a necessary and sufficient condition for the ability to violate the CHSH inequality. Experimentally it can be realized by randomized measurements which can approximate its value arbitrarily closely. This makes it independent of a shared reference frame between the two measuring parties, which can be useful in scenarios where it is impossible to find one. In this second article, we show that average correlation also serves as an indicator for inseparability by deriving a necessary and sufficient condition. From there, we prove the remaining open conjectures of the first article. Due to the operational definition of average correlation, it offers a first step toward finding a new operationally defined inseparability measure.

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I. INTRODUCTION

Entanglement, that is, inseparability of quantum states, is one of the defining features of quantum physics which sets it apart from classical physics. Over the last decades, inseparability has become the basis for many quantum technologies [1] such as quantum communication [2], quantum computing [3] and quantum sensing [4]. While inseparability is defined in terms of the structure of quantum states in Hilbert space, in practice we observe it by nonclassical correlations in an experiment, which manifest themselves by the violation of Bell inequalities [5–11].

One of the most prominent examples of these inequalities is the Clauser-Horne-Shimony-Holt (CHSH) inequality [6,12]

$$S(\mathbf{a},\mathbf{a}';\mathbf{b},\mathbf{b}') \equiv |E(\mathbf{a},\mathbf{b}) + E(\mathbf{a}',\mathbf{b}) + E(\mathbf{a},\mathbf{b}') - E(\mathbf{a}',\mathbf{b}')| \leqslant 2, \tag{1}$$

which is based on four different correlation functions

$$E(\mathbf{a},\mathbf{b}) \equiv \mathrm{tr}(\hat{\rho}\,\mathbf{a}\cdot\hat{\boldsymbol{\sigma}}_A \otimes \mathbf{b}\cdot\hat{\boldsymbol{\sigma}}_B), \tag{2}$$

with the density operator of the two-qubit state $\hat{\rho}$, as well as the vectors of the Pauli operators $\hat{\boldsymbol{\sigma}}_A = (\hat{\sigma}_{1A}, \hat{\sigma}_{2A}, \hat{\sigma}_{3A})$ and $\hat{\boldsymbol{\sigma}}_B = (\hat{\sigma}_{1B}, \hat{\sigma}_{2B}, \hat{\sigma}_{3B})$ for two distant observers A and B measured along the measurement axes $\mathbf{a}$ and $\mathbf{a}'$ for observer A and $\mathbf{b}$ and $\mathbf{b}'$ for observer B. Finding the optimal measurement settings which allow for a violation of the CHSH inequality requires accurate measurements and a shared reference frame with which both observers A and B can align their measurements [13]. In practice, however, coordinating measurements and especially finding a shared reference frame can become challenging.

One way of circumventing this problem is to use reference frame independent quantities [14], especially using randomized measurements [15–26], that is, measuring quantities, such as correlation functions with randomized measurement settings. The advantage of such measurements is that the outcome does then not depend on the measurements, but is now only state-dependent.

In the last few years, many quantities based on randomized measurements have been proposed and tested experimentally [26]. Such quantities often allow testing inseparability. Whether and how often a Bell inequality is violated in particular is however more challenging. One way is to evaluate CHSH inequalities for many randomly chosen measurements and check how often the CHSH inequality is violated [15–17].

While this method avoids a shared reference frame, it still requires both parties to coordinate their measurements and to revisit earlier measurements, as each party has to perform every measurement twice; see Eq. (1). As such, it does not allow for a completely randomized approach, nor can both parties randomize independently.

This problem can be addressed by using average correlation [27], which is also reference frame independent but based on fully and independently randomized measurements, and

[*]michael.tschaffon@uni-ulm.de
[†]johannes.seiler@uni-ulm.de

serves as an indicator for nonclassicality in the Bell sense [28]. We have shown that a necessary and sufficient condition based on the value of average correlation exist, that allow us to predict, whether the state can violate the CHSH inequality.

Beyond the derivation of a necessary and sufficient condition for a violation of the CHSH inequality, we have demonstrated numerically that for each value of average correlation Σ a minimal and maximal value for the Bell parameter s, that is, the maximum of the CHSH inequality,

$$s \equiv \max S(\mathbf{a}, \mathbf{a}'; \mathbf{b}, \mathbf{b}'), \tag{3}$$

can be reached, allowing us to map out all states in a $\Sigma - s$ map. While the minimal value and thus the lower boundary in the map could be shown to be defined by Werner states, the maximal value or upper boundary could only be derived for values $\Sigma \leqslant 1/4$. For values $\Sigma > 1/4$ it could only be conjectured that pure states deliver the maximal Bell parameter. Furthermore, while numerical simulations suggest that many states could be found between these fundamental boundaries, it was not shown whether the $\Sigma - s$ map could be filled completely, that is, whether there exist states for every pair of values of Σ and s between the upper and lower boundary.

In this article, we show that average correlation provides not only an indicator for nonclassicality of states, but even directly indicates inseparability of the state. To do so, we address the two open problems described above, one by one. In particular, we first summarize the essential results with regard to average correlation and formulate the open questions in detail in Sec. II. We then address these questions by first showing in Sec. III that the positivity condition presents restrictions on the different correlation matrices. In Sec. IV, we then use these criteria to derive a necessary and sufficient condition for inseparability. Moreover, in Sec. V, we demonstrate that pure states indeed possess the maximal Bell parameter for $\Sigma > 1/4$. Finally, in Sec. VI we prove that every point in the $\Sigma - s$ map corresponds to a physical state. To keep our article self-contained but focused on the main ideas, we present detailed calculations in two appendices. In Appendix A we prove the inseparability conditions, while in Appendix B we show in detail that the $\Sigma - s$ map can be filled completely.

II. AVERAGE CORRELATION

In this article we primarily study the nonclassicality indicator average correlation [27]

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

which is defined as the modulus of the correlation function, Eq. (2), averaged over all possible measurement directions $\mathbf{a}$ and $\mathbf{b}$. To evaluate this quantity we note that any bipartite qubit state can be written in the Fano form [29]

$$\hat{\rho} = \frac{1}{4}\left(\hat{\mathbb{1}} + \mathbf{q}\cdot\hat{\boldsymbol{\sigma}}_A \otimes \hat{\mathbb{1}}_B + \hat{\mathbb{1}}_A \otimes \mathbf{r}\cdot\hat{\boldsymbol{\sigma}}_B + \sum_{ij} K_{ij}\hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}\right), \tag{5}$$

containing the local Bloch vectors $\mathbf{q}$ and $\mathbf{r}$ as well as the correlation matrix K with real elements

$$K_{ij} = \mathrm{tr}(\hat{\rho}\, \hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}). \tag{6}$$

For the correlation matrix we can perform a singular value decomposition [13]

$$K = U \kappa V^T, \tag{7}$$

with orthogonal matrices U and V and a diagonal matrix κ which only contains the singular values α, β and γ with $1 \geqslant \alpha \geqslant \beta \geqslant \gamma \geqslant 0$.

Since we average over all measurement directions $\mathbf{a}$ and $\mathbf{b}$, average correlation Σ only depends on the singular values α, β and γ or likewise on α, γ and the Bell parameter

$$s = 2\sqrt{\alpha^2 + \beta^2}. \tag{8}$$

We define a state to be nonclassical if there exists at least one way of constructing a CHSH inequality, Eq. (1), such that the inequality is violated. In other words, a state is nonclassical if its maximal value of the CHSH inequality, that is, the Bell parameter s, is greater than 2.

As we have laid out in Ref. [27], average correlation is a suitable indicator for nonclassicality, as defined above, for three reasons. For one, it is only state dependent since we average over all measurement directions and therefore only depends on the correlation matrix of a state. In addition, it indicates nonclassicality as there is both a necessary, $\Sigma > 1/4$, and a sufficient condition, $\Sigma > 1/(2\sqrt{2})$, for nonclassicality. In other words, if a state has a value of average correlation higher than $\Sigma = 1/4$, then it can be nonclassical while a value higher than $\Sigma = 1/(2\sqrt{2})$ guarantees that the state is nonclassical. Last, it is defined operationally, which enables an experimental translation. To theoretically study Σ and s, it suffices to study the singular values of the correlation matrix.

However, finding the singular values for a general correlation matrix K is not always straight forward. Thus, as a next step to simplify calculations for the following sections, we perform a basis change. We choose our computational basis in a way such that K becomes diagonal. For this purpose, we recall [30] that for every unitary matrix $\hat{\mathcal{U}}$ exists a unique rotation O such that $\hat{\mathcal{U}}(\mathbf{r}\cdot\hat{\boldsymbol{\sigma}})\hat{\mathcal{U}}^\dagger = (O\,\mathbf{r})\cdot\hat{\boldsymbol{\sigma}}$ for all Euclidean vectors $\mathbf{r}$. If we choose two such unitary transformations $\hat{\mathcal{U}}_A$ and $\hat{\mathcal{U}}_B$ for our basis change for subsystems A and B, that is, we define $|0'\rangle_{A/B} = \hat{\mathcal{U}}_{A/B}|0\rangle_{A/B}$ and $|1'\rangle_{A/B} = \hat{\mathcal{U}}_{A/B}|1\rangle_{A/B}$, in such a way that the resulting rotations O_1 and O_2 diagonalize the correlation matrix according to

$$K' = O_1\, K\, O_2^\dagger, \tag{9}$$

then we can rewrite the corresponding quantum state $\hat{\rho}$ in the new basis as

$$\hat{\rho} = \frac{1}{4}\left(\hat{\mathbb{1}} + \mathbf{q}'\cdot\hat{\boldsymbol{\sigma}}'_A \otimes \hat{\mathbb{1}}_B + \hat{\mathbb{1}}_A \otimes \mathbf{r}'\cdot\hat{\boldsymbol{\sigma}}'_B + \sum_{i} K'_i\hat{\sigma}'_{iA} \otimes \hat{\sigma}'_{iB}\right), \tag{10}$$

where $\mathbf{q}' = O_1\mathbf{q}$ and $\mathbf{r}' = O_2\mathbf{r}$, and $K'_i = K'_{ii}$ are the diagonal and thus only nonzero elements of K'. The diagonal elements of K' are, up to a sign, identical to the singular values α, β and γ, as O_1 and O_2 are rotations, that is, $\det O = 1$, and not general orthogonal matrices as needed in the singular value decomposition. As a consequence, the sign of the determinant of K is preserved and the diagonal elements of K' are not necessarily all positive, as it is the case with κ in the singular value decomposition, Eq. (7). For simplicity, we drop the primes for the remainder of this article.

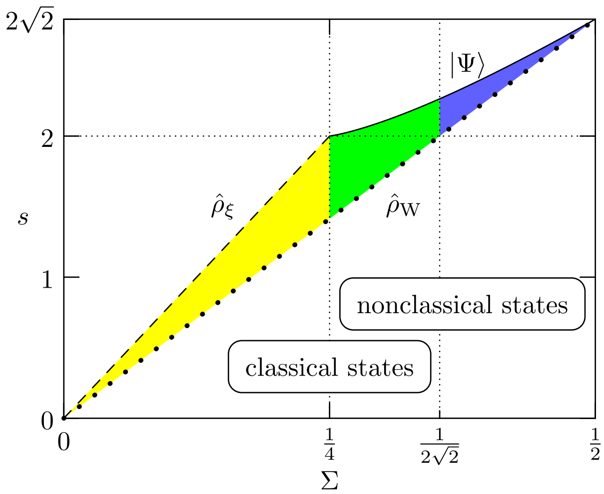

FIG. 1. Bell parameter s as a function of average correlation Σ for pure states $|\Psi\rangle$ (solid line), Werner states $\hat{\rho}_W$ (dotted line) and ξ states $\hat{\rho}_\xi$ (dashed line). All physical states are conjectured to be within these three classes of states. For $\Sigma < 1/4$, colored in yellow, we only find classical states, i.e., $s \leqslant 2$, while for $\Sigma > 1/(2\sqrt{2})$, colored in blue, we only find nonclassical states, i.e., $s > 2$. In between these two values for Σ, colored in green, we find both classical and nonclassical states.

To better understand how the Bell parameter s and average correlation Σ relate, we study all two-qubit states in a $\Sigma - s$ map, as shown in Fig. 1. There we have plotted analytically three classes of states: Pure states $|\Psi\rangle$, Werner states $\hat{\rho}_W$ [31], and ξ states [27,32]

$$\hat{\rho}_\xi = \frac{1+\xi}{2}|1\rangle\langle 1|_A \otimes |0\rangle\langle 0|_B + \frac{1-\xi}{2}|0\rangle\langle 0|_A \otimes |0\rangle\langle 0|_B. \tag{11}$$

A numerical [33] simulation of randomly generated states shows that all the states are found inside these three classes of states in the $\Sigma - s$ map [27]. Thus, we have conjectured that they define the boundaries in this map. Indeed, the lower boundary, that is, the Werner states, as well as the upper boundary in the nonclassical regime, i.e., the ξ states have been shown [27]. As depicted in the plot, all states in between these two boundaries are classical, i.e., they have a Bell parameter $s < 2$, if they do not satisfy the necessary condition for nonclassicality, $\Sigma > 1/4$, colored in yellow, while they are nonclassical if they satisfy the sufficient condition $\Sigma > 1/(2\sqrt{2})$, colored in blue. All states in between these two values, colored in green, can be either classical or nonclassical.

Despite all of these findings, there are still a number of limitations. Even though we can make many exact theoretical statements about average correlation, experimentally, the value of average correlation can only be approximated by measuring randomly very often and thus practically evaluating the integral in Eq. (4). While the accuracy increases with the number of measurements, we are still dealing with a finite number of measurements and not with infinitely many as it would theoretically be required. As such, the value of average correlation can fundamentally never be measured, but only a quantity approximating it. On top of this, randomization in theory has to occur for the measurement direction uniformly, that is, evenly over the surface of the Bloch sphere. In the experiment, however, this could be challenging, as a randomization over the involved parameters does not necessarily give one an even distribution of the measurement directions in which case it would have to be adjusted and thus not completely randomized anymore.

Aside from the experimental limitations, we still have many unaddressed challenges with regard to generalizing average correlation, that is, when we go beyond two-qubit states. If we try to define average correlation with respect to more than two parties, then nonclassicality cannot be defined in terms of the CHSH inequality anymore, as it strictly deals with bipartite correlations. Hence, a different definition would have to be found. If we employ states other than qubit states, then we cannot construct the CHSH inequality in a straightforward manner as it requires a dichotomic observable, so one would have to be artificially introduced, e. g. a quantity of a subspace of the larger Hilbert space like a pseudo spin.

However, apart from the aforementioned challenges which are inherently part of the nature of average correlation, two unsolved questions stand out most. First, as already raised above, the upper boundary in the nonclassical regime has not been proven but only been motivated numerically. This means it is not clear if pure states are truly the upper boundary. Second, even though states in all regions of the $\Sigma - s$ map have been found, it has not been proven that there is a state for every point in the map within the boundaries. In other words, it has to be shown, that physical states completely fill the map.

The first problem, that is, the fact that we cannot get above pure states in the $\Sigma - s$ map, is in fact related to positivity of the states, as states above this boundary would not be positive. This will be examined in more detail in the next section.

III. POSITIVITY

Positivity of the state $\hat{\rho}$ requires that the inequalities [30]

$$1 + K_3 \pm (K_1 - K_2) \geqslant 0 \tag{12}$$

and

$$1 - K_3 \pm (K_1 + K_2) \geqslant 0 \tag{13}$$

containing the diagonal elements K_1, K_2 and K_3 of the diagonalized correlation matrix K hold. When we take into consideration the different signs that the diagonal elements can have, we can distinguish two cases. For one, if the diagonalized correlation matrix K has three negative diagonal elements, then Eqs. (12) and (13) are rewritten as

$$1 - |K_3| \pm (|K_2| - |K_1|) \geqslant 0 \tag{14}$$

and

$$1 + |K_3| \pm (|K_2| + |K_1|) \geqslant 0. \tag{15}$$

Furthermore, one negative sign, no matter for which diagonal element, and two positive signs yield the same four inequalities as just derived, albeit in a different order. As pointed out in the last section, up to a sign the diagonal elements of K are identical to the singular values α, β, and γ of K. If in the first equation we either set $|K_1|$ or $|K_2|$ equal to γ or in the second equation $|K_3|$ equal to γ, then we arrive at

$$\gamma \geqslant \alpha + \beta - 1, \tag{16}$$

along with inequalities which are trivially satisfied.

If, however, we have three positive diagonal elements, then we instead arrive at the inequalities

$$1 + |K_3| \pm (|K_1| - |K_2|) \geqslant 0 \tag{17}$$

and

$$1 - |K_3| \pm (|K_1| + |K_2|) \geqslant 0, \tag{18}$$

which also result from one positive and two negative diagonal elements. No matter which diagonal element corresponds to which singular value, the last two inequalities yield the only nontrivial condition

$$1 \geqslant \alpha + \beta + \gamma, \tag{19}$$

which is an even stricter inequality than Eq. (16). While the inequality above only has to be fulfilled for certain signs, Eq. (16) is always valid and is thus the only nontrivial inequality which has to be satisfied due to positivity. Hence, we refer to this condition as the positivity condition. Note that the positivity condition gives us a minimal value for γ other than zero.

We emphasize that for one negative or three negative signs we arrived at an even tighter condition, Eq. (19), which is in fact along with the minimal value of γ related to inseparability, as we will explore in the next section.

IV. INSEPARABILITY

A bipartite state is defined as separable if it can be written as a convex sum [31]

$$\hat{\rho} = \sum_k p_k \, \hat{\varrho}_{kA} \otimes \hat{\varrho}'_{kB} \tag{20}$$

of tensor products of one particle states $\hat{\varrho}_{kA}$ and $\hat{\varrho}'_{kB}$ with probabilities p_k. A two-qubit state is separable if and only if its partial transpose is nonnegative [34]. It was shown [35] that this is precisely the case when the trace norm $||K||$ of the correlation matrix of the state is less than or equal to one, that is,

$$||K|| = \alpha + \beta + \gamma \leqslant 1. \tag{21}$$

As we have seen in the last section, positivity leads to a condition, Eq. (19), identical to the separability condition above, if we have two negative or three positive diagonal elements in the diagonalized correlation matrix. This makes two negative or three positive diagonal elements of the diagonalized correlation matrix K a sufficient condition for separability.

Further, we note that if a state is separable, that is, the above inequality is satisfied, Eq. (16) is automatically satisfied. Consequently, γ can be arbitrarily small and the minimal value of γ is given by zero while for inseparable states it is given by

$$\gamma \geqslant \alpha + \beta - 1 \tag{22}$$

and thus greater than zero.

Now that we know how the minimal value for γ is related to inseparability, we will as a final point address the question for what values of Σ we find separable and for what values inseparable states. It is already known that inseparability is a necessary condition for nonclassicality. Further, we know that for $\Sigma > 1/4$ states can be nonclassical. As we show in Appendix A, $\Sigma = 1/4$ is not only the necessary condition for nonclassicality but also the sufficient condition for inseparability. But what about a necessary condition? For that we require the smallest possible value of Σ for which the separability condition, Eq. (19), barely holds, i.e., $\alpha + \beta + \gamma = 1$. In Appendix A, we show that this value is given by $\Sigma = 1/6$, making $\Sigma > 1/6$ a necessary condition for inseparability.

In fact, $\Sigma = 1/6$ is the value for which Werner states become inseparable, which makes it the class of states which are inseparable for the lowest possible value of average correlation Σ. However, at the same time, they are also the class of states which are nonclassical for the highest possible value of $\Sigma = 1/2\sqrt{2}$. Pure states behave exactly opposite to this. They are nonclassical for the lowest possible value but also inseparable for the highest possible value, both at $\Sigma = 1/4$ [27]. This again emphasizes our view that Werner states are the most classical states as the difference between their values of Σ for which they are inseparable and nonclassical is maximal, while pure states are the most nonclassical states as there is no difference.

Now that we have derived a minimal value for γ as a result of the positivity of the underlying state and demonstrated how it is related to inseparability, we apply this knowledge in the next section to derive an upper boundary in the inseparable regime, that is, $\Sigma > 1/4$. As we will see in the next section, it is inseparability which makes the upper boundary a different class of states for the separable and inseparable regime.

V. UPPER BOUNDARY

To derive the upper boundary in the $\Sigma - s$ map, we have to minimize average correlation $\Sigma = \Sigma(\alpha, s, \gamma)$ as a function of the Bell parameter s with respect to the singular values α and γ. In Ref. [27] it was shown that for a given value of the Bell parameter s, average correlation Σ is monotonically decreasing in α and monotonically increasing in γ and thus minimal for a minimal value of γ and a maximal value of α. Thus, the minimal value of γ plays a crucial role in the upper boundary. However, as shown in the last section, this minimal value depends on whether the underlying state is separable or inseparable. Thus, we will distinguish these two cases.

For a separable state, that is, $\alpha + \beta + \gamma \leqslant 1$, γ can be as small as zero. So, to minimize Σ, we set $\gamma = 0$. As for α, we note from Eq. (8) that it can maximally be half of the Bell parameter s but other than for $s = 2$ cannot be equal to one, as this would make the state inseparable. Hence, using the definition of the Bell parameter Eq. (8), we get a minimal average correlation for the singular values $\alpha = s/2$, $\beta = 0$ and $\gamma = 0$. This condition corresponds to ξ states $\hat{\rho}_\xi$ with $\xi = s/2$, which was already derived in Ref. [27].

In the inseparable regime $\Sigma > 1/4$, the lowest value for γ is, due to the positivity condition Eq. (16), given by $\gamma = \alpha + \beta - 1$. However, for nonclassical states, $s > 2$, α can be as large as one. To minimize Σ, we set $\alpha = 1$ which then immediately gives us $\gamma = \beta$. Using Eq. (8) once again, we then obtain $\beta = \sqrt{(s/2)^2 - \alpha^2} = \sqrt{(s/2)^2 - 1}$. Hence, in the inseparable regime, that is, for $\Sigma > 1/4$, average correlation Σ becomes minimal for a given value of the Bell parameter s, and thus corresponds to the upper boundary in the $\Sigma - s$ map, for singular values $\alpha = 1$, $\beta = \gamma = \sqrt{(s/2)^2 - 1}$. This corresponds to pure states as conjectured before [27].

We note that it is precisely the fact that the smallest possible value of γ is different in the different regimes, which gives rise to the kink in Fig. 1 where product states are found. If we move along the boundary corresponding to the smallest values for γ, i.e., the upper boundary, then positivity requires that there is a kink once the states are inseparable, which is why it is exactly the product states which are found at the kink.

However, there is one last question that needs to be answered. Even if all states are found between the three fundamental boundaries in the $\Sigma - s$ map, can we assign every pair of Σ and s values a physical state, that is, is the area between the boundaries completely filled? We investigate this final open question in the next section.

VI. QUANTUM CHANNELS

If we want to obtain values for average correlation and the Bell parameter for all states, then it is sufficient to consider all possible singular values of a correlation matrix, as average correlation and the Bell parameter only depend on them.

To do so, we consider a model where we start with the maximally entangled Bell state $|\Psi^{(-)}\rangle$ and subject it to a quantum channel consisting of three fundamental errors on each subsystem: a bit flip, a bit-phase flip, and a phase flip, represented by the three Pauli operators $\hat{\sigma}_1$, $\hat{\sigma}_2$, and $\hat{\sigma}_3$, respectively. We mathematically describe this quantum channel using the Kraus operators [36–38]

$$\hat{M}_j = c_j \, \hat{\sigma}_{jA} \otimes \hat{\mathbb{1}}_B \tag{23}$$

with complex coefficients c_j and $\hat{\sigma}_{0A} \equiv \hat{\mathbb{1}}_A$ satisfying the completeness relation

$$\sum_{j=0}^{3} \hat{M}_j^\dagger \hat{M}_j = \hat{\mathbb{1}}. \tag{24}$$

As a result of this quantum channel, the Bell state $|\Psi^{(-)}\rangle$ is mapped to a mixture

$$\hat{\rho} = \sum_{j=0}^{3} \hat{M}_j |\Psi^{(-)}\rangle\langle\Psi^{(-)}| \hat{M}_j^\dagger = \sum_{k\in\{\Psi^{(\pm)},\Phi^{(\pm)}\}} p_k(\lambda, p) |k\rangle\langle k| \tag{25}$$

of the four Bell states

$$|\Psi^{(\pm)}\rangle \equiv \tfrac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle) \tag{26}$$

and

$$|\Phi^{(\pm)}\rangle \equiv \tfrac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \tag{27}$$

with probabilities p_k which are identical to the absolute value square of the complex coefficients c_j in the definition of the Kraus operators, Eq. (23), that is $p_{\Psi^{(-)}} = |c_0|^2$ and so on. This model is useful, as the four Bell states all have diagonal correlation matrices in the computational basis, with absolute values of the diagonal elements equal to one but with different signs; see Appendix B. As such, this approach allows us to construct a state with specific singular values depending on our choice of the probabilities p_k. But what does the action of the individual errors physically mean, and how does it relate to the boundaries? To better understand this, we consider two extreme cases.

In the first case, we initially let only one error act on the Bell state, that is, we have $p_{\Psi^{(\pm)}} = (1 \mp p)/2$ and $p_{\Phi^{(\pm)}} = 0$. As a consequence, the Bell state is then mapped to

$$\hat{\rho} = \frac{1+p}{2} |\Psi^{(-)}\rangle\langle\Psi^{(-)}| + \frac{1-p}{2} |\Psi^{(+)}\rangle\langle\Psi^{(+)}|, \tag{28}$$

i.e., a decohering Bell state which has the same singular values and consequently the same value for average correlation as a pure state. In fact, here, the channel is a dephasing channel for decreasing values of p [36]. Then, as a second step we subject the completely decohered Bell state, $p = 0$, to a different error, now with $p_{\Psi^{(-)}} = (1+\lambda)/2$ and $p_{\Phi^{(-)}} = (1-\lambda)/2$, and end up with a state

$$\hat{\rho} = \frac{\lambda}{2}(|01\rangle\langle 01| + |10\rangle\langle 10|) + \frac{1-\lambda}{4}\mathbb{1}, \tag{29}$$

which for $\lambda = 1$ is equivalent to the product state but then for decreasing values of λ finally reaches the completely mixed state, equivalent to ξ states $\hat{\rho}_\xi$ [27,32].

Alternatively, in the other case, we set $p_{\Psi^{(-)}} = (1+3\lambda)/4$ and $p_{\Psi^{(+)}} = p_{\Phi^{(+)}} = p_{\Phi^{(-)}} = (1-\lambda)/4$, that is all three fundamental errors equally large, and let $\lambda \in [0, 1]$ decrease, giving us a Werner state [31]

$$\hat{\rho} = \lambda |\Psi^{(-)}\rangle\langle\Psi^{(-)}| + \frac{1-\lambda}{4}\mathbb{1} = \hat{\rho}_{\mathrm{W}}(\lambda). \tag{30}$$

This makes our channel a depolarizing channel [36] which for λ approaching zero directly maps the state to the completely mixed state.

The difference between these two situations is that in the former case we have first acted with one error, the phase flip, giving us a specific channel, the dephasing channel, which initially leaves the state nonclassical, i.e., $s > 2$. Only by applying the other error, the bit flip, in a second step, the state becomes nonclassical, corresponding to first pure states and then ξ states and thus moving along the upper boundary of the $\Sigma - s$ map. In contrast, in the latter case, the state experienced all three errors at once, i.e., the depolarizing channel, mapping it to Werner states and as such moving along the lower boundary from the Bell state all the way to the completely mixed state, too. So, with the quantum channel model described above, the upper and lower boundary obtain a physical meaning. They correspond to different ways of a Bell state decohering to the completely mixed state. Both situations are depicted in Fig. 2.

For every other state in between the two boundaries, we note that we can reach any point in the map if we make the choice

$$p_{\Psi^{(\pm)}} = \frac{1 + \lambda(1 \mp 2p)}{4}, \tag{31}$$

and

$$p_{\Phi^{(\pm)}} = \frac{1-\lambda}{4} \tag{32}$$

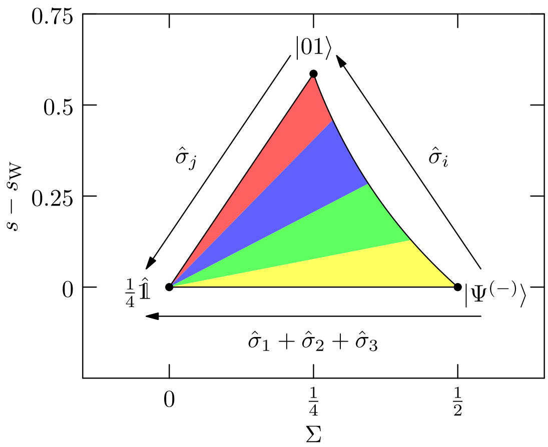

FIG. 2. Difference between the Bell parameter s and the Bell parameter for Werner states s_W as a function of average correlation Σ. One of the Bell states $|\Psi^{(-)}\rangle$, one of the product states $|01\rangle$ and the completely mixed state $\hat{\mathbb{1}}/4$ are marked by large dots. Every state on the upper boundary can be represented by a Bell state experiencing first one error, here $\hat{\sigma}_i$, and then experiencing a different error, here $\hat{\sigma}_j$ with $i, j \in \{1, 2, 3\}$. States on the lower boundary can be represented by a Bell state experiencing all three errors at once, i.e., $\hat{\sigma}_1$, $\hat{\sigma}_2$, and $\hat{\sigma}_3$. Bell states that have experienced the error $\hat{\sigma}_3$ with a probability $[1 + \lambda(1 - 2p)]/4$ and the other two errors with a probability $(1 - \lambda)/4$ for different values of $\lambda \in [0, 1]$ are colored in yellow for $p \in [1, 0.75)$, in green for $p \in [0.75, 0.5)$, in blue for $p \in [0.5, 0.25)$ and in red for $p \in [0.25, 0]$. For a fixed value of p, states are situated along a straight line connecting the completely mixed state ($\lambda = 0$) to a pure state ($\lambda = 1$) with concurrence p, where the gradient of the line is fixed by the parameter p and the proximity to the pure states is closer for larger values of λ. The smaller the value for p is the closer the straight line is to the upper boundary between the product state and the completely mixed state corresponding to ξ states, which have the value $p = 0$, while $p = 1$ corresponds to the lower boundary, that is, Werner states.

with the two visibilities $\lambda \in [0, 1]$ and $p \in [0, 1]$, as we show in Appendix B. In this parametrization, the former route along the upper boundary corresponds to first setting $\lambda = 1$ and decreasing p, and then setting $p = 0$ and decreasing λ [39], while the latter route corresponds to setting $p = 1$ and decreasing λ. Any different combination of λ and p values gives rise to a state in between the boundaries, completely filling the map, as depicted in Fig. 2. As we show in detail in Appendix B, this is because for a fixed value of p we start at the completely mixed state in the map for $\lambda = 0$ and then for increasing values of λ move along a straight line to a pure state with concurrence [40] p for $\lambda = 1$. The gradient of the straight line is determined by p such that for $p = 1$ the straight line corresponds to Werner states and then for decreasing values of p approaches the line for ξ states for $p = 0$. In this way, the $\Sigma - s$ map can be filled completely, as seen in Fig. 2, where areas with different values of p are shaded in different colors.

Accordingly, any state in between the upper and lower boundary can be viewed as a quantum channel which is somewhere in between these two different scenarios, with some having a more dominant error making them closer to the upper boundary, while others have more similarly large errors making them closer to the lower boundary, depending on the exact choice of the parameters λ and p.

TABLE I. Necessary and sufficient conditions for inseparability and nonclassicality with respect to the value of average correlation Σ for two-qubit states.

Condition	Value of Σ
Necessary condition for inseparability	$\Sigma > 1/6$
Sufficient condition for inseparability	$\Sigma > 1/4$
Necessary condition for nonclassicality	$\Sigma > 1/4$
Sufficient condition for nonclassicality	$\Sigma > 1/(2\sqrt{2})$

VII. CONCLUSIONS AND OUTLOOK

In summary, we have derived two new inequalities for average correlation with regard to inseparability. Namely, for $\Sigma > 1/6$ we can have inseparable states while for $\Sigma > 1/4$ we must have inseparable states, making these two values a necessary and a sufficient condition for inseparability and as such average correlation an indicator for inseparability. The necessary and sufficient conditions for inseparability, derived in this article, and nonclassicality, derived in Ref. [27], are summarized in Table I.

We have used these results to finally show that indeed in the inseparable regime, i.e., $\Sigma > 1/4$, the upper boundary of the $\Sigma - s$ map is given by pure states, that is we find no class of states with a higher Bell parameter s for a given value of average correlation. Last, we were able to show that the $\Sigma - s$ map can be filled completely with states, that is for every pair of values of Σ and s between the three fundamental boundary states, at least one state can be found.

Despite these results, there are still open questions. For one, it will be interesting to explore whether and how average correlation can be generalized to states other than two-qubit states and if we can find similar results regarding nonclassicality and inseparability. Further, comparing average correlation to other measures based on randomized measurements and checking whether additional information can be obtained by using the combined information of average correlation and these measures could yield more insights.

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APPENDIX A: CONDITIONS FOR INSEPARABILITY

In this Appendix, we derive a necessary and sufficient condition for inseparability of two-qubit states based on average correlation.

To do so, we will first derive the extreme of average correlation for fixed values of $\alpha + \beta + \gamma = c$, then derive the minimum and maximum and show how the minimum and maximum give rise to the necessary and sufficient condition for inseparability.

1. Stationary points

We need to find stationary points, that is, extreme values of average correlation $\Sigma(\alpha,\beta,\gamma)$ under the constraint $\alpha+\beta+\gamma=c$. This problem can be addressed using Lagrange multipliers. We start out by defining the Lagrangian function

$$\Lambda(\alpha,\beta,\gamma,\chi)=\Sigma(\alpha,\beta,\gamma)+\chi(c-\alpha-\beta-\gamma) \quad \text{(A1)}$$

involving average correlation, which is to be minimized or maximized, and a term that has to vanish under the above-mentioned constraint multiplied by a Lagrange multiplier χ. An extreme value under this constraint appears if the gradient of the Lagrangian function with respect to all variables vanishes. This is precisely the case if all derivatives

$$\frac{\partial\Sigma}{\partial\alpha}=\frac{\partial\Sigma}{\partial\beta}=\frac{\partial\Sigma}{\partial\gamma}=\chi, \quad \text{(A2)}$$

with respect to all variables evaluated at the stationary point equate to the multiplier χ. As such, we need to find points for which the derivatives with respect to the singular values become equal.

To find these points, we rewrite average correlation [27]

$$\Sigma(\alpha,\beta,\gamma)=\frac{\alpha}{4}\left\{1+\frac{1}{2\pi}\int_0^{2\pi}d\phi\, g[f(\phi)]\right\}, \quad \text{(A3)}$$

with the functions

$$g[f(\phi)]=\frac{f(\phi)}{\sqrt{1-f(\phi)}}\mathrm{Arsinh}\left(\sqrt{\frac{1-f(\phi)}{f(\phi)}}\right) \quad \text{(A4)}$$

and

$$f(\phi)=\left(\frac{\beta}{\alpha}\right)^2\sin^2\phi+\left(\frac{\gamma}{\alpha}\right)^2\cos^2\phi. \quad \text{(A5)}$$

The derivatives with respect to the singular values then evaluate to

$$\begin{aligned}\frac{\partial\Sigma}{\partial\alpha}&=\frac{1}{4}+\frac{1}{8\pi}\int_0^{2\pi}d\phi\left\{g[f(\phi)]+\alpha g'[f(\phi)]\frac{\partial f}{\partial\alpha}\right\}\\&=\frac{1}{4}+\frac{1}{8\pi}\int_0^{2\pi}d\phi\{g[f(\phi)]-2g'[f(\phi)]f(\phi)\}, \quad \text{(A6)}\end{aligned}$$

$$\begin{aligned}\frac{\partial\Sigma}{\partial\beta}&=\frac{\alpha}{8\pi}\int_0^{2\pi}d\phi\, g'[f(\phi)]\frac{\partial f}{\partial\beta}\\&=\frac{1}{4\pi}\int_0^{2\pi}d\phi\, g'[f(\phi)]\frac{\beta}{\alpha}\sin^2\phi, \quad \text{(A7)}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial\Sigma}{\partial\gamma}&=\frac{\alpha}{8\pi}\int_0^{2\pi}d\phi\, g'[f(\phi)]\frac{\partial f}{\partial\gamma}\\&=\frac{1}{4\pi}\int_0^{2\pi}d\phi\, g'[f(\phi)]\frac{\gamma}{\alpha}\cos^2\phi\\&=\frac{1}{4\pi}\int_0^{2\pi}d\phi\, g'[(\gamma/\alpha)^2\sin^2\phi+(\beta/\alpha)^2\cos^2\phi]\\&\quad\times\frac{\gamma}{\alpha}\sin^2\phi, \quad \text{(A8)}\end{aligned}$$

where in the last step we have performed the substitution $\phi\to\phi+\pi/2$ and rearranged integration domains and g' denotes the derivative of g with respect to f. The last two derivatives are identical, except that the roles of β and γ are interchanged. These two derivatives are then obviously equal if we choose $\beta=\gamma$, which then yields a constant function

$$f=\left(\frac{\beta}{\alpha}\right)^2, \quad \text{(A9)}$$

making g independent of ϕ and enabling us to evaluate the integrals resulting in the derivatives

$$\left.\frac{\partial\Sigma}{\partial\beta}\right|_{\beta=\gamma}=\left.\frac{\partial\Sigma}{\partial\gamma}\right|_{\beta=\gamma}=\frac{1}{4\pi}\frac{\beta}{\alpha}g'\int_0^{2\pi}d\phi\sin^2\phi=\frac{1}{4}\sqrt{f}g' \quad \text{(A10)}$$

and

$$\left.\frac{\partial\Sigma}{\partial\alpha}\right|_{\beta=\gamma}=\frac{1}{4}(1+g-2fg'). \quad \text{(A11)}$$

Finally, if we want all derivatives to be equal, then we have to equate the two equations above and arrive at the differential equation

$$\frac{1}{4}\sqrt{f}g'=\frac{1}{4}(1+g-2fg'), \quad \text{(A12)}$$

which is in general not solved by $g(f)$ and thus only satisfied by certain values of f. To find these values, we rewrite the derivative of $g(f)$ [27]

$$\begin{aligned}g'&=\frac{2-f}{2\sqrt{1-f}^3}\mathrm{Arsinh}\left(\sqrt{\frac{1-f}{f}}\right)-\frac{1}{2(1-f)}\\&=\frac{1}{2(1-f)}\left[\left(\frac{2}{f}-1\right)g-1\right], \quad \text{(A13)}\end{aligned}$$

as a function of $g(f)$ itself. By inserting Eq. (A13) into Eq. (A12) and solving the resulting equation for g, we arrive at the condition

$$g(f)=\frac{f+2\sqrt{f}}{2\sqrt{f}+2-f}\equiv h(f), \quad \text{(A14)}$$

in which the functions $g(f)$ and $h(f)$ must be equal for a given value of $f\in(0,1)$. The values one and zero, however, have to be treated in the limit, as f and $f-1$ appear in denominators in Eqs. (A12) and (A13).

To find solutions to the above equation, we note that the second-order derivative of $h(f)$ given by

$$h''(f)=\frac{2-2\sqrt{f}^3-3f^2-3f+6\sqrt{f}}{\sqrt{f}^3(f-2\sqrt{f}-2)^3} \quad \text{(A15)}$$

is clearly negative and $h(f)$ thus concave on the interval. For g we find for the second-order derivative

$$\begin{aligned}g''=\frac{1}{4(1-f)^2}&\left\{2\left[\left(\frac{2}{f}-1\right)g-1\right]\right.\\&\left.+2(1-f)\left[\left(\frac{2}{f}-1\right)g'-\frac{2}{f^2}g\right]\right\}. \quad \text{(A16)}\end{aligned}$$

Inserting Eq. (A13) into this equation and rearranging terms, we see that the second-order derivative of g is negative if

$$(f-4)g > -(f+2) \tag{A17}$$

holds. From Ref. [27] we recall that $g(f) \geqslant f(5+f)/6$. Thus, the inequality above is true if we have

$$\frac{f}{6}(5+f)(f-4) > -(f+2), \tag{A18}$$

which is indeed satisfied on the interval $(-1-\sqrt{13}, 1)$ and thus for $f \in (0, 1)$. Hence, both functions $h(f)$ and $g(f)$ are concave for $f \in (0, 1)$ and are therefore equal for two values of f at most. These two values are given by $f = 0$ and $f = 1$ as it can be seen immediately that we have $h(0) = 0$ and $h(1) = 1$ which agrees with the limit $g \to 0$ for $f \to 0$ and $g \to 1$ for $f \to 1$, respectively [27]. However, as we have noted before, Eq. (A14) is only valid on the open interval $f \in (0, 1)$ and therefore a solution on this interval does not exist. For the remaining values of one and zero, we have to check whether Eq. (A12) is satisfied in the limit $f \to 0$ and $f \to 1$, respectively.

For $f \to 0$ we get

$$\lim_{f\to 0} fg' = \lim_{f\to 0} \frac{f}{2(1-f)}\left[\left(\frac{2}{f}-1\right)g-1\right] = 0, \tag{A19}$$

which when inserted into Eq. (A12) together with the limit $g \to 0$ for $f \to 0$ requires the limit of $\sqrt{f}g'$ to approach one in order for both sides of the equation to become equal. However, using l'Hospital's rule, we see that this limit

$$\begin{aligned}\lim_{f\to 0} \sqrt{f}g' &= \lim_{f\to 0} \frac{\sqrt{f}}{2(1-f)}\left[\left(\frac{2}{f}-1\right)g-1\right]\\ &= \lim_{f\to 0} \frac{(2-f)g}{2\sqrt{f}(1-f)} = \lim_{f\to 0} \frac{(2-f)g'-g}{(1-f)/\sqrt{f}-2\sqrt{f}}\\ &= 2\lim_{f\to 0} \sqrt{f}g'\end{aligned} \tag{A20}$$

is identical to twice itself and thus cannot be equal to one [41]. This means that Eq. (A12) is not solved in the limit $f \to 0$.

In the limit $f \to 1$ we find using l'Hospital's rule and the fact that we have $g \to 1$ for $f \to 1$ [27] that the derivative of g given by Eq. (A13) approaches

$$\lim_{f\to 1} g' = \lim_{f\to 1}\left[\frac{g}{f^2}+\left(\frac{1}{2}-\frac{1}{f}\right)g'\right] = 1 - \frac{1}{2}\lim_{f\to 1} g', \tag{A21}$$

and we thus solve it algebraically by

$$\lim_{f\to 1} g' = \tfrac{2}{3}. \tag{A22}$$

By inserting this limit, as well as the limit $g \to 1$ into Eq. (A12), we see that both sides of the equation approach the same value 1/6 and it is therefore solved in the limit $f \to 1$ making it the unique solution of Eq. (A12).

Consequently, for $\beta = \gamma$ the Lagrangian function becomes stationary only in the limit $f \to 1$, that is, for $\alpha = \beta$, and thus for three equally large singular values $\alpha = \beta = \gamma = c/3$. Since this is the only local extreme, this means that due to the monotony of the function this has to be a global extreme as well. However, which type of global extreme it is, is yet to be determined, which we will do in the next subsection.

2. Minimum

To find out what type of extreme we have, we have to examine the signs of the third and fourth principal minor of the bordered Hessian [42]

$$H(\alpha,\beta,\gamma) = \begin{pmatrix} 0 & \frac{\partial^2\Lambda}{\partial\alpha_j\partial\chi} \\ \frac{\partial^2\Lambda}{\partial\alpha_i\partial\chi} & \frac{\partial^2\Lambda}{\partial\alpha_i\partial\alpha_j}\end{pmatrix}, \tag{A23}$$

with $\alpha_i, \alpha_j \in \{\alpha, \beta, \gamma\}$, that is, the Hessian of the Lagrangian function $\Lambda(\alpha, \beta, \gamma, \chi)$, evaluated at the stationary point $\alpha = \beta = \gamma = c/3$ and as such in the limit $f \to 1$.

To do so, using Eq. (A1), we first compute the derivatives

$$\frac{\partial^2\Lambda}{\partial\alpha\partial\chi} = \frac{\partial^2\Lambda}{\partial\beta\partial\chi} = \frac{\partial^2\Lambda}{\partial\gamma\partial\chi} = -1, \tag{A24}$$

with respect to the singular values and the Lagrange multiplier χ, which are all equal and independent of f. As a next step, we evaluate the second-order derivatives

$$\left.\frac{\partial^2\Lambda}{\partial\alpha^2}\right|_{\beta=\gamma} = \frac{1}{2\alpha}[f\,g'(f) + 2f^2\,g''(f)], \tag{A25}$$

$$\left.\frac{\partial^2\Lambda}{\partial\alpha\partial\beta}\right|_{\beta=\gamma} = -\frac{1}{4\alpha}[2\,g''(f)\sqrt{f}f + g'(f)\sqrt{f}] = \left.\frac{\partial^2\Lambda}{\partial\alpha\partial\gamma}\right|_{\beta=\gamma}, \tag{A26}$$

$$\left.\frac{\partial^2\Lambda}{\partial\beta^2}\right|_{\beta=\gamma} = \frac{1}{4\alpha}\left[g'(f) + \frac{3}{2}f\,g''(f)\right] = \left.\frac{\partial^2\Lambda}{\partial\gamma^2}\right|_{\beta=\gamma}, \tag{A27}$$

and

$$\left.\frac{\partial^2\Lambda}{\partial\beta\partial\gamma}\right|_{\beta=\gamma} = \frac{1}{8\alpha}f\,g''(f), \tag{A28}$$

with respect to the singular values at the stationary point, which, using $\alpha = c/3$, gives us the final contribution

$$\begin{aligned}\left(\frac{\partial^2\Lambda}{\partial\alpha_i\partial\alpha_j}\right) &= \frac{3}{4c}g'(f)\begin{pmatrix} 2f & -\sqrt{f} & -\sqrt{f} \\ -\sqrt{f} & 1 & 0 \\ -\sqrt{f} & 0 & 1\end{pmatrix}\\ &\quad + \frac{3}{8c}f\,g''(f)\begin{pmatrix} 8f & -4\sqrt{f} & -4\sqrt{f} \\ -4\sqrt{f} & 3 & 1 \\ -4\sqrt{f} & 1 & 3\end{pmatrix}\end{aligned} \tag{A29}$$

to the bordered Hessian, involving the first-order and second-order derivatives of g with respect to f.

Finally, to perform the limit $f \to 1$, we have to find the limit of the second-order derivative g''. To do so, we apply l'Hospital's rule in Eq. (A16) and make use of $g \to 1$ and $g' \to 2/3$, see Eq. (A22), for $f \to 1$. The limit then becomes

$$\begin{aligned}\lim_{f\to 1} g'' &= -\frac{1}{4}\lim_{f\to 1}\left[\left(\frac{2}{f}-1\right)g'' - \frac{4}{f^2}g' + \frac{4}{f^3}g\right]\\ &= -\frac{1}{4}\lim_{f\to 1} g'' - \frac{1}{3}\end{aligned} \tag{A30}$$

and can be algebraically solved, equating to $-4/15$.

We are now in a position to evaluate the bordered Hessian at the stationary point. For $\alpha = c/3$ and in the limit $f \to 1$, the bordered Hessian approaches

$$\lim_{f\to 1} H(\alpha = c/3, \beta, \gamma) = \frac{1}{10c}\begin{pmatrix} 0 & -10c & -10c & -10c \\ -10c & 2 & -1 & -1 \\ -10c & -1 & 2 & -1 \\ -10c & -1 & -1 & 2 \end{pmatrix}, \tag{A31}$$

which has the third principal minor

$$\det\left[\frac{1}{10c}\begin{pmatrix} 0 & -10c & -10c \\ -10c & 2 & -1 \\ -10c & -1 & 2 \end{pmatrix}\right] = -\frac{3}{5c} \tag{A32}$$

and the fourth principal minor

$$\det\left[\frac{1}{10c}\begin{pmatrix} 0 & -10c & -10c & -10c \\ -10c & 2 & -1 & -1 \\ -10c & -1 & 2 & -1 \\ -10c & -1 & -1 & 2 \end{pmatrix}\right] = -\frac{27}{100c^2}, \tag{A33}$$

which are both negative. This makes the point $\alpha = \beta = \gamma = c/3$ a local and, as discussed before, the global minimum of the Lagrangian function [42]. This point corresponds to Werner states, which makes the average correlation

$$\Sigma = \frac{c}{6} \tag{A34}$$

of the lower boundary of the $\Sigma - s$ map the minimal value of average correlation for which $c = \alpha + \beta + \gamma$ is satisfied. In particular, this makes the value $\Sigma = 1/6$ the lowest possible value to barely satisfy the separability condition $c \leqslant 1$, making

$$\Sigma > \tfrac{1}{6} \tag{A35}$$

a necessary condition for inseparability.

So far, using Lagrange multipliers, we have found a minimum. Since this minimum is the only local extreme, the global maximum has to be found at the boundary of the parameter space. Finding the maximum will be the task of the next subsection.

3. Maximum

The boundary of the parameter space is reached by either setting α equal to one or γ equal to zero. In the following, we distinguish between the inseparable, i.e., $c > 1$, and separable regime, i.e., $c \leqslant 1$.

When we are in the inseparable regime, we cannot set γ equal to zero and thus need to set α equal to one. Then due to the positivity condition, Eq. (16), γ has to be equal to β. This corresponds to pure states with $\beta = \gamma = (c-1)/2$.

In the separable regime, α cannot be one, and we thus need to set γ equal to zero. The resulting average correlation then reads [27]

$$\Sigma(\alpha, \beta, \gamma = 0) = \frac{\alpha}{4} E(k = \sqrt{1 - \beta^2/\alpha^2}), \tag{A36}$$

where $E(k)$ is the complete elliptic integral of the second kind. The above equation is identical to the sixteenth of the perimeter of an ellipse with semimajor axis α and semiminor axis β [43]. To find the maximum, we note that an ellipse with semiaxes α and β is enclosed by a rectangle with side lengths 2α and 2β, see Fig. 3, that is, its perimeter is never greater than the perimeter of the enclosing rectangle given by $4\alpha + 4\beta$. The maximal value of average correlation for $\gamma = 0$ is thus found by finding the ratio of semiaxes of an ellipse whose perimeter is closest to that of the enclosing rectangle with fixed perimeter.

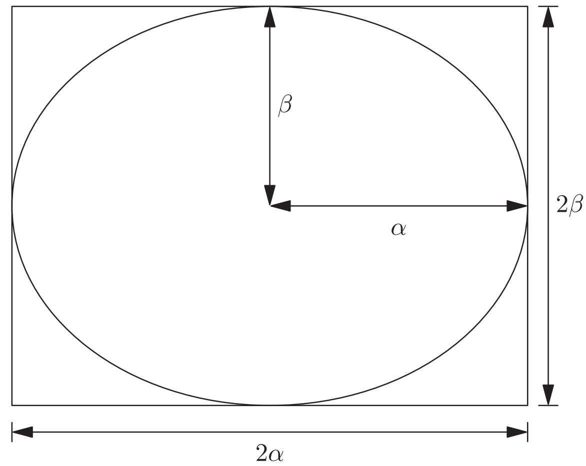

FIG. 3. Ellipse with semimajor axis α and semiminor axis β enclosed by a rectangle with side lengths 2α and 2β. The perimeter of the ellipse is always less than the perimeter of the rectangle except for $\beta = 0$, for which they become equal.

We note that the perimeter of the ellipse becomes identical to its enclosing rectangle, and is thus maximal, for $\beta = 0$, that is, the ellipse and the rectangle both degenerate to twice a line with length $2\alpha = 2c$; see Fig. 3.

Hence, in the separable regime for $\alpha + \beta + \gamma = c$, average correlation becomes maximal for $\alpha = c$ and $\beta = \gamma = 0$, which is precisely the value of average correlation for ξ states

$$\Sigma = \frac{c}{4} \tag{A37}$$

with $\xi = c$.

So, both in the separable and inseparable regime, the maximal value of average correlation for a fixed value of $c = \alpha + \beta + \gamma$ is found by setting α maximal and β and γ minimal. This corresponds to ξ states in the separable and to pure states in the inseparable regime, and thus to the upper boundary in the $\Sigma - s$ map.

The maximal value for which we can still find separable states, that is, $c = 1$, is thus given by

$$\Sigma = \tfrac{1}{4}, \tag{A38}$$

making $\Sigma > 1/4$ a sufficient condition for inseparability.

APPENDIX B: FILLING THE $\Sigma - s$ MAP

In this Appendix, we show that the $\Sigma - s$ map can be filled completely, that is, for each pair of values of average correlation Σ and Bell parameter s between the upper and lower boundary we can find a state. For this purpose, we consider the $\lambda - p$ states

$$\hat{\rho}_{\lambda p}(\lambda, p) = \sum_{k\in\{\Psi^{(\pm)},\Phi^{(\pm)}\}} p_k(\lambda, p)|k\rangle\langle k| = \lambda\left(\frac{1+p}{2}|\Psi^{(-)}\rangle\langle\Psi^{(-)}| + \frac{1-p}{2}|\Psi^{(+)}\rangle\langle\Psi^{(+)}|\right) + \frac{1-\lambda}{4}\hat{\mathbb{1}}, \tag{B1}$$

with the Bell states

$$|\Psi^{(\pm)}\rangle \equiv \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle) \tag{B2}$$

and

$$|\Phi^{(\pm)}\rangle \equiv \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \tag{B3}$$

as well as the probabilities

$$p_{\Psi^{(\pm)}}(\lambda, p) = \frac{1+\lambda(1\mp 2p)}{4} \tag{B4}$$

and

$$p_{\Phi^{(\pm)}}(\lambda, p) = \frac{1-\lambda}{4}. \tag{B5}$$

To examine the behavior of this class of states in the $\Sigma - s$ map, we need to find the singular values of its correlation matrix $K_{\lambda p}$, Eq. (6). For this purpose, we make use of the linearity of the correlation matrix

$$(K_{\lambda p})_{ij} = \mathrm{tr}\left[\left(\sum_{k\in\{\Psi^{(\pm)},\Phi^{(\pm)}\}} p_k|k\rangle\langle k|\right)\hat{\sigma}_{iA}\otimes\hat{\sigma}_{jB}\right] = \sum_{k\in\{\Psi^{(\pm)},\Phi^{(\pm)}\}} p_k \mathrm{tr}(|k\rangle\langle k|\hat{\sigma}_{iA}\otimes\hat{\sigma}_{jB}) = \sum_{k\in\{\Psi^{(\pm)},\Phi^{(\pm)}\}} p_k (K_k)_{ij} \tag{B6}$$

and the correlation matrices of the Bell states

$$K_{\Psi^{(\pm)}} = \mathrm{diag}(\pm 1, \pm 1, -1) \tag{B7}$$

and

$$K_{\Phi^{(\pm)}} = \mathrm{diag}(\pm 1, \mp 1, 1) \tag{B8}$$

to derive the correlation matrix

$$K_{\lambda p} = \frac{1+\lambda(1+2p)}{4}K_{\Psi^{(-)}} + \frac{1-\lambda}{4}K_{\Phi^{(-)}} + \frac{1+\lambda(1-2p)}{4}K_{\Psi^{(+)}} + \frac{1-\lambda}{4}K_{\Phi^{(+)}} = -\mathrm{diag}(\lambda p, \lambda p, \lambda) \tag{B9}$$

of the $\lambda - p$ states with singular values $\alpha = \lambda$, $\beta = \lambda p$, and $\gamma = \lambda p$. The Bell parameter for this class of states is thus given by

$$s = 2\sqrt{\alpha^2+\beta^2} = 2\lambda\sqrt{1+p^2}. \tag{B10}$$

As a final step, we need to compute average correlation [27]

$$\Sigma = \frac{\alpha}{4}\left[1 + \frac{1}{2\pi}\int_0^{2\pi} d\phi\, \frac{f(\phi)}{\sqrt{1-f(\phi)}}\mathrm{Arsinh}\left(\sqrt{\frac{1-f(\phi)}{f(\phi)}}\right)\right]. \tag{B11}$$

With the help of the singular values, we find that the function

$$f(\phi) = p^2, \tag{B12}$$

Eq. (A5), is independent of ϕ. As a consequence, average correlation of $\lambda - p$ states immediately evaluates to

$$\Sigma_{\lambda p} = \frac{\lambda}{4}\left[1 + \frac{p^2}{\sqrt{1-p^2}}\mathrm{Arsinh}\left(\frac{\sqrt{1-p^2}}{p}\right)\right]. \tag{B13}$$

We note that if we set $\lambda = 1$, we end up with the average correlation of pure states [27] with a concurrence p, while if we fix p and use the Bell parameter given by Eq. (B10), we can rewrite it to

$$\Sigma_{\lambda p} = \frac{s}{8\sqrt{1+p^2}}\left[1 + \frac{p^2}{\sqrt{1-p^2}}\mathrm{Arsinh}\left(\frac{\sqrt{1-p^2}}{p}\right)\right], \tag{B14}$$

making it linear in the Bell parameter s with a gradient that is larger for increasing values of p. For $p = 0$, average correlation then becomes $\Sigma_{\lambda p} = s/8$ and thus equal to ξ states, while for $p = 1$ it evaluates to $\Sigma_{\lambda p} = s/(4\sqrt{2})$ and hence equal to Werner states [27]. For a general value of $p \in [0, 1]$, its average correlation is a line extending from the completely mixed state, that is, $\Sigma = 0$ and $s = 0$, to the upper boundary given by pure states with concurrence p, that is, Eq. (B13) with $\lambda = 1$.

Since the value for p can be chosen arbitrarily in the interval $p \in [0, 1]$, the $\lambda - p$ states completely fill the $\Sigma - s$ map. Hence, for each pair of values of average correlation Σ and Bell parameter s between the upper and lower boundary, we find at least one state.

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