

Pearson correlation coefficient as a measure for certifying and quantifying high-dimensional entanglement

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A scheme for characterizing entanglement using the statistical measure of correlation given by the Pearson correlation coefficient (PCC) was recently suggested that has remained unexplored beyond the qubit case. Towards the application of this scheme for the high-dimensional states, a key step has been taken in a very recent work by experimentally determining PCC and analytically relating it to Negativity for quantifying entanglement of the empirically produced bipartite pure state of spatially correlated photonic qutrits. Motivated by this work, we present here a comprehensive study of the efficacy of such an entanglement characterizing scheme for a range of bipartite qutrit states by considering suitable combinations of PCCs based on a limited number of measurements. For this purpose, we investigate the issue of necessary and sufficient certification together with quantification of entanglement for the two-qutrit states comprising maximally entangled state mixed with white noise and colored noise in two different forms, respectively. Further, by considering these classes of states for $d = 4$ and 5 , extension of this PCC-based approach for higher dimensions (d) is discussed.

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I. INTRODUCTION

Seminal discoveries of the applications of quantum entanglement in cryptography [1], superdense coding [2], and teleportation [3] have given rise to a rich body of works that have demonstrated the remarkable power of entanglement as resource for quantum communication and information processing tasks, ranging from secure key distribution [4], quantum computational speed-up [5], reduction of communication complexity [6,7], to device-independent certification of genuine randomness [8,9]. These explorations have primarily focused on considering the two-dimensional (qubit) systems. Alongside, though, it is important to note that there have been a number of studies indicating a range of advantages gained by using high-dimensional entangled states, for example, achieving more robust quantum key distribution protocols with higher key rate [10–13], ensuring increased security of the device independent key distribution protocols against even tiny imperfection in randomness generation [14], enhancing quantum communication channel capacity [15,16], as well as lowering the rate of entanglement decay arising from atmospheric turbulence in the context of free-space quantum communication [17] and reducing the critical detection efficiency required for more robust tests of quantum nonlocality [18].

Thus, in light of this promising potentiality of high-dimensional entangled states, the characterization of such experimentally produced entangled states is of much significance. Here it needs to be noted that the tomographic characterization of quantum states is constrained by the requirement to determine a large number of independent parameters depending upon the dimension of the system [19]. Hence, in order to obviate this difficulty, the study of characterization of high-dimensional entangled states based on a limited number of measurements has been attracting an increasing attention. Further, since which of the proposed schemes for characterizing entanglement would be most readily amenable to experimental implementation is *a priori* an open question, the search for various effective schemes on this issue acquires considerable significance. It is in this context, the present paper seeks to systematically investigate the formulation of a scheme for the characterization of high-dimensional entanglement based on a well-known statistical measure of correlation known as the Pearson correlation coefficient. In order to set the appropriate backdrop for this work, we first briefly recall the relevant important studies to date.

On the one hand, there are schemes making use of entanglement witnesses to provide lower bounds on the entanglement measures [20,21], on the other hand, operational quantification of entanglement in a measurement-device-independent way has been analyzed within the context of a subclass of semiquantum nonlocal games [22] and this approach has been used [23] to provide measurement-device-independent bounds on entanglement quantifiers like Negativity. Also, of particular interest in this context are the recent studies [24–26] formulating approaches to provide sufficient characterization of bipartite high-dimensional entanglement

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based on determining a lower bound to the entanglement of formation from a limited number of measurements. Among these approaches, the scheme used by Bavaresco *et al.* [26] gives an optimal estimate of the lower bound for entanglement of formation, and this scheme is easier to experimentally implement because it involves only two local measurements in each wing of the bipartite system. A different approach [27] based on the violation of entropic inequalities witnessing steerability of high-dimensional entanglement with only two local measurements, too, has been shown to provide an optimal lower bound to the entanglement of formation.

However, all such approaches focusing essentially on providing bounds on entanglement measures do not provide quantification of entanglement in terms of determining the actual value of an entanglement measure like entanglement of formation or Negativity. On the other hand, while the characterization of entanglement for bipartite and multipartite qubit states was earlier discussed in terms of appropriate inequalities involving Bell correlations [28], a recent relevant study [29] proposes using the Son-Lee-Kim (SLK) inequality (a bipartite Bell-type inequality whose violation can show nonlocality of high-dimensional states) for entanglement characterization by relating the nonzero value of the measurable SLK function to Negativity (concurrence) in the case of high-dimensional pure states (isotropic mixed states) based on measurements of an appropriately chosen set of observables. However, this approach has the limitation that nonzero value of the SLK function is not a sufficient condition for certifying entanglement since there are separable mixed states for which the SLK function is nonzero for the measurements of the observables specified in this approach. Now, while such approaches make use of linear inequalities, there have also been studies [30,31] formulating nonlinear entanglement witnesses that are more effective in detecting entanglement than the linear entanglement witnesses, however, still not quantifying entanglement in the sense mentioned earlier.

Next, considering the other approaches that have been proposed for the characterization of entanglement for high-dimensional bipartite systems, the following are particularly noteworthy. A scheme based on the sum of mutual information using two mutually unbiased bases (MUBs) has been invoked to certify various noisy mixed entangled states in higher-dimensional cases using the notion that a bipartite multidimensional state in even dimension can be regarded as an ensemble of bipartite qubit states [32]; however, this scheme provides only a sufficient criterion for detecting entanglement and quantifies entanglement in terms of entanglement of formation, essentially restricted to the maximally entangled state [33]. Another approach based on the notion of mutual predictability has led to the argument that the condition of the sum of mutual predictabilities pertaining to MUBs exceeding a certain bound can serve as a necessary and sufficient criterion for certifying entanglement of pure and isotropic mixed states in any dimension [34]. On the other hand, using measurements pertaining to correlations present in two appropriately chosen MUBs, the experimental feasibility of a scheme [35] has been argued that can determine essentially a lower bound to the entanglement of formation for any state,

while providing only sufficient certification of entanglement of the colored-noise and isotropic mixed states.

The preceding discussion, thus, underscores the lack of schemes that, apart from necessary and sufficient certification, can also quantify high-dimensional entanglement in the sense of determining the actual value of an appropriate entanglement measure in terms of a limited number of experimentally measurable quantities. Of course, in such analyses, it is assumed at the outset that the empirical procedure for preparing a bipartite correlated state can specify it to be pure or mixed, and if mixed, the type of noise that is involved in the preparation procedure. The approach we adopt here is based on analytically linking an empirically accessible statistical measure of correlation with a suitable entanglement measure. For this purpose, Maccone *et al.* [33] had suggested the use of Pearson correlation coefficient [36] for entanglement characterization. The Pearson correlation coefficient (PCC) for any two random variables A and B is defined as

$$C_{AB} \equiv \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle}{\sqrt{\langle A^2 \rangle - \langle A \rangle^2} \sqrt{\langle B^2 \rangle - \langle B \rangle^2}}, \quad (1)$$

whose values can lie between -1 and 1 , and $\langle \cdot \rangle$ is an average value. Note that although PCC is a well known measure of correlation that has been applied extensively in different areas of statistical applications, surprisingly, it has so far been used in physics only in a few cases such as for quantifying the temporal correlation between classical trajectories in the context of synchronization problems [37], for the quantification of synchronization in the context of temporal dynamics of local observables of a bipartite quantum system [38], and for formulating a Bell-CHSH-type inequality in terms of PCCs [39].

Now, let us explore the application of PCC in the context of the following scenario: suppose a bipartite pure or mixed state of the given dimension d is shared between Alice and Bob; Alice (Bob) performs two d -outcome measurements $A_1 (B_1)$ and $A_2 (B_2)$ on her (his) subsystem. Then, for $A_1 = B_1 = \sum_j a_j |a_j\rangle \langle a_j|$ and $A_2 = B_2 = \sum_j b_j |b_j\rangle \langle b_j|$, where $\{|a_j\rangle\}$ is mutually unbiased to $\{|b_j\rangle\}$, the following condition has been conjectured by Maccone *et al.* to certify entanglement of bipartite systems:

$$|C_{A_1 B_1}| + |C_{A_2 B_2}| > 1, \quad (2)$$

which is postulated to imply entanglement. However, this procedure based on PCCs has been applied for entanglement characterization restricted to *only* the qubits [33].

In this context, it is important to take note of the line of studies that has been recently initiated by measuring PCCs for a bipartite photonic qutrit pure state which has been produced using a novel pump beam modulation-based technique [40]. Subsequently, very recently, by analytically relating the experimentally measurable quantity PCC with Negativity as a measure of entanglement, the value of Negativity for the empirically prepared nearly maximally entangled state has been inferred, thereby constituting the first work using PCC demonstrating entanglement detection and quantification beyond the two-qubit case [41]. While in that work, specifically, pure two-qutrit states have been considered, in this paper we embark on a comprehensive study of the application of

PCC-based entanglement characterizing scheme. In particular, we explore the above mentioned conjecture of Maconné *et al.* by considering a range of mixed states like isotropic and two-types of colored-noise mixed states, as well as the Werner and Werner-Popescu states in terms of the sum of suitable number of PCCs.

Here it is relevant to note that the particular significance of the qutrit systems stems from the considerable practical advantages as compared to qubits that have been decisively shown in the context of quantum cryptography [42], quantum computation [43], and robustness against entanglement decay [17]; moreover, because of the intriguing nature of the relationship that has been pointed out for the qutrits between the magnitude of violation of Bell-type inequality and the amount of entanglement [44–46], the study of entangled qutrits acquires an added fundamental significance.

A salient feature of our treatment worth stressing is that it is the idea of Negativity as a measure of entanglement that turns out to be useful for relating it to PCCs in a way that enables effective characterization of entanglement for the classes of states considered in this paper. Here it is relevant to recall that introduction of the idea of Negativity by Życzkowski *et al.* [47] stimulated its use as an entanglement measure through demonstration that it is an entanglement monotone for any finite-dimensional bipartite entangled state [48]. Later, applications of this quantity, defining it as the absolute value of the sum of negative eigenvalues of partial transposed density matrix, were pointed out in different contexts like relating its lower bound to the violations of Bell-CHSH inequality and steering inequality, respectively, [49,50]. A physical meaning of Negativity has been provided by arguing that Negativity can be viewed as an estimator of the number of degrees of freedom of the two subsystems that are entangled, as well as can be viewed as determining in a device-independent way the minimum number of dimensions that contribute to the quantum correlation [51]. In this context, the relationship between Negativity and PCCs found in this paper can have interesting implications revealing further aspects of the physical meaning of Negativity for higher dimensional systems.

Now, let us summarize the salient results obtained in Sec. II for the *qutrit* case:

(a) We consider maximally entangled state mixed with white noise in two different forms, *isotropic mixed states* [52–54] and *Werner-Popescu states* [52,55]. For both these classes of mixed states, it is found that by appropriately choosing four mutually noncommuting bases which are *not* MUBs, the sum of four PCCs being greater than 1 provides the *necessary* and *sufficient condition* for certifying entanglement, as well as the *quantification* of entanglement is obtained through an analytically derived *monotonic relation* in terms of *Negativity*.

(b) We consider two types of *colored noise* mixed with a maximally entangled state. In one of the types, a colored-noise state having perfect correlation in the computational basis is mixed with the maximally entangled state [32]. For this family of states, we find that one can choose two appropriate MUBs so that the sum of two PCCs being greater than 1 gives the *necessary* and *sufficient condition* for certifying entanglement;

quantification of entanglement is also obtained similar to the earlier cases in terms of *Negativity*.

In the other type, a colored-noise state having anticorrelation in the computational basis is mixed with the maximally entangled state [56]. For this class of states, we find that for the appropriately chosen four mutually noncommuting bases which are not MUBs, the sum of four PCCs being greater than 1 furnishes the *certification and quantification* of entanglement, provided *Negativity is nonvanishing*.

(c) Considering the entanglement characterization of *Werner state* [57], which, in any arbitrary dimension, is a mixture of projectors onto the antisymmetric subspace and white noise in the higher dimensional case, it turns out that by using the sets of four appropriate mutually noncommuting bases, MUBs as well as non-MUBs, we can show the sum of four PCCs to be providing a *sufficient criterion* for the certification of entanglement, as well as the *quantification* of entanglement can be achieved by relating it to *Negativity*.

It is thus evident that for the effective characterization of entanglement using PCCs for the different types of qutrit mixed states, the number of measurements suffice to be limited to either only two or four MUBs or noncommuting bases. An interesting point to note is that while the schemes for efficient tomography and those invoking the notions of mutual information and mutual predictability usually use MUBs, the approach proposed for entanglement characterization in terms of PCCs can work for some specific classes of states like isotropic mixed states, a type of colored-noise, Werner, and Werner-Popescu states, even using mutually noncommuting bases that are not MUBs. This is similar to the case of nonlocality studies using Bell-type inequalities involving measurements pertaining to mutually noncommuting bases which do not necessarily need to be MUBs [46]. Here we may also mention that apart from its other applications, the procedure of entanglement characterization and quantification using PCCs in the qutrit case, together with the results of studies on the nonlocality of bipartite qutrit states can provide a powerful experimental platform for a comprehensive probing of hitherto unexplored quantitative aspects of the relationship between entanglement and nonlocality [44–46,58–63].

In Sec. III towards exploring the potentiality of this method for higher dimensions $d > 3$, the results of studies probing extension of this scheme for the dimensions $d = 4$ and 5 will be discussed, in particular, for the pure as well as the isotropic, two types of colored-noise, Werner, and Werner-Popescu mixed states (see Fig. 1 which gives a schematic outline of this entanglement characterization approach). We now proceed to delve into the specifics, beginning with the case of isotropic mixed states.

II. TWO-QUTRIT STATES

A. Isotropic mixed states

Let us begin by writing the general expression for the two-qutrit isotropic mixed state [52–54] given by

$$\rho_I(F) = \frac{1-F}{d^2-1} (\mathbb{1} - |\phi_d^+\rangle\langle\phi_d^+|) + F |\phi_d^+\rangle\langle\phi_d^+|, \quad (3)$$

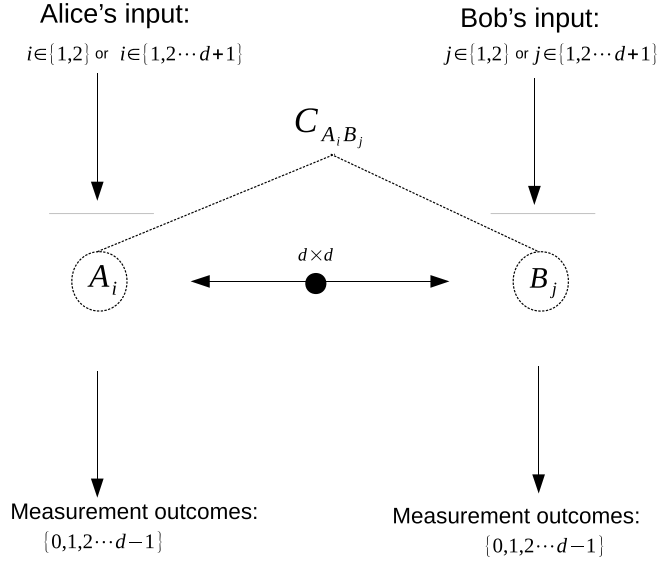


FIG. 1. Entanglement characterization approach based on the sum of Pearson correlation coefficients (PCCs). Two experimentalists, Alice and Bob, have access to the subsystems of a bipartite $d \times d$ quantum system. Alice and Bob perform two or $d + 1$ local measurements in mutually unbiased bases or noncommuting bases. From the measurement statistics, Alice and Bob can check whether the sum of two PCCs given by $C_{A_1 B_1} + C_{A_2 B_2}$ (in the case of pure states) or the sum of $d + 1$ PCCs given by $\sum_{i,j=1}^{d+1} C_{A_i B_j}$ (in the case of mixed states) is greater than 1 to determine whether the given bipartite quantum state is entangled or not.

where $F = \langle \phi_d^+ | F | \phi_d^+ \rangle$ satisfying $0 \leq F \leq 1$ is the fidelity of $\rho_I(F)$ and

$$|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |i\rangle \otimes |i\rangle, \quad (4)$$

which is the maximally entangled state in dimension d and \mathbb{I} is the identity matrix of dimension $d \times d$. For the two-qudit isotropic mixed state $\rho_I(p)$, Negativity as defined in Ref. [48] can be computed from the partial transposed density matrix and is given by

$$\mathcal{N}(\rho_I(F)) = \max \left\{ \frac{dF - 1}{2}, 0 \right\}, \quad (5)$$

which is nonzero if and only if $F > 1/d$. Interestingly, it turns out that the two-qudit isotropic mixed state $\rho_I(F)$ is entangled if and only if the same condition is satisfied, *viz.*, $F > 1/d$ [52]. Therefore, it follows that the Negativity of this class of states as given by Eq. (5) provides the necessary and sufficient quantification of entanglement for any d .

For our purpose here for the necessary as well as sufficient certification of entanglement, we now construct the following set of four noncommuting bases which are not MUBs:

$$\begin{aligned} \{|a_j\rangle\} &= \{|0\rangle, |1\rangle, |2\rangle\}, \\ \{|b_j\rangle\} &= \{(|0\rangle + |1\rangle + |2\rangle)/\sqrt{3}, \\ &(|0\rangle + \omega |1\rangle + \omega^2 |2\rangle)/\sqrt{3}, \\ &(|0\rangle + \omega^2 |1\rangle + \omega |2\rangle)/\sqrt{3}\}, \end{aligned}$$

$$\begin{aligned} \{|e_j\rangle\} &= \{(|0\rangle + e^{i\pi/3} |1\rangle + e^{2i\pi/3} |2\rangle)/\sqrt{3}, \\ &(|0\rangle - |1\rangle + |2\rangle)/\sqrt{3}, \\ &(|0\rangle + \omega^2 e^{i\pi/3} |1\rangle + \omega e^{2i\pi/3} |2\rangle)/\sqrt{3}\}, \\ \{|g_j\rangle\} &= \{(\omega^2 |0\rangle + \omega |1\rangle - |2\rangle)/\sqrt{3}, \\ &(|0\rangle + |1\rangle - |2\rangle)/\sqrt{3}, \\ &(\omega |0\rangle + \omega^2 |1\rangle - |2\rangle)/\sqrt{3}\}, \end{aligned} \quad (6)$$

where $\omega = e^{2i\pi/3}$. Here, the eigenvalues a_j of the computational basis [64] are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, the second basis $\{|b_j\rangle\}$ corresponds to what we call the generalized σ_x basis (with the eigenvalues $b_0 = 0$, $b_1 = +1$, $b_2 = -1$), the third basis $\{|e_j\rangle\}$ corresponds to what we call the generalized σ_y basis (with the eigenvalues $b_0 = +1$, $b_1 = 0$, $b_2 = -1$), and the eigenvalues g_j of the fourth basis are given by $g_0 = +1$, $g_1 = 0$, and $g_2 = -1$.

Here we may remark that what we call the generalized $\hat{\sigma}_x$ and the generalized $\hat{\sigma}_y$ bases mentioned above which will be used later are obtained from the general expression for the d -dimensional basis invoked by Scarani *et al.* [65] in the context of studies related to the CGLMP inequality, and also used in the treatment by Spengler *et al.* [34]. This eigenbasis $\{\Psi_x(a)\}$ of a d -dimensional observable as invoked by these authors can be written in terms of the computational basis as

$$\Psi_x(a) \equiv \sum_{k=0}^{d-1} \frac{e^{i(2\pi/d)ak}}{\sqrt{d}} (e^{ik\phi_x} |k\rangle), \quad (7)$$

where $a = 0, 1, 2, \dots, (d-1)$ label the different eigenvectors. For $d \geq 3$, we call the basis $\{\Psi_x(a)\}$ with $\phi_x = 0$ and $\phi_x = \pi/d$ the generalized σ_x basis and the generalized σ_y basis respectively. This terminology is used in the sense that in the case of $d = 2$, the above expression reduces to the eigenbases corresponding to σ_x and σ_y observables, respectively.

Next, using the earlier mentioned bases given by Eq. (6), we find that the necessary and sufficient certification of entanglement for the two-qudit isotropic states can be obtained in terms of the sum of four PCCs $\sum_{i=1}^4 |C_{A_i B_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle \langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle \langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle \langle e_j|$, and $A_4 = B_4 = \sum_j g_j |g_j\rangle \langle g_j|$, whence the sum of these four PCCs is given by

$$\sum_{i=1}^4 |C_{A_i B_i}| = \frac{|9F - 1|}{2} > 1 \quad \text{iff} \quad F > 1/3. \quad (8)$$

See Appendix A for the derivation of the above expression for the sum of four PCCs. Now, from Eqs. (5) and (8) it follows that since, as mentioned earlier, the two-qudit isotropic mixed state is entangled if and only if $F > 1/3$ whence Negativity is nonzero, the sum of four PCCs as given above being greater than 1 provides necessary and sufficient certification of entanglement. Next, we argue that the sum of PCCs given by Eq. (8) also provides quantification of certified entanglement of the two-qudit isotropic states in the following sense.

Now, note that using Eq. (5), one can write Negativity of the two-qudit isotropic mixed state for $F > 1/3$:

$$\mathcal{N}(\rho_I(F)) = \frac{3F - 1}{2}. \quad (9)$$

From Eq. (9), using Eq. (8) it follows that for $F > 1/3$

$$\sum_{i=1}^4 |C_{A_i B_i}| = 1 + 3\mathcal{N}(\rho_I(F)). \quad (10)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

B. Colored noise mixed with maximally entangled state

Here we consider two families of two-qutrit mixed states having maximally entangled state mixed with two types of colored noise. In one of them (labeled A), a colored-noise state has perfect correlation in the computational basis and in the other type (labeled B), a colored-noise state has perfect anticorrelation in the computational basis.

Colored-noise mixed states-A. Let us write the general expression for the colored-noise two-qudit maximally entangled state, which is a mixture of the two-qudit maximally entangled state $|\phi_d^+\rangle$ and the colored-noise two-qudit state $1/d \sum_{i=0}^{d-1} |ii\rangle\langle ii|$ given by

$$\rho_{cc}(p) = p|\phi_d^+\rangle\langle\phi_d^+| + \frac{(1-p)}{d} \sum_{i=0}^{d-1} |ii\rangle\langle ii|, \quad (11)$$

where p is the mixed parameter, $0 \leq p \leq 1$. In Ref. [32] experimental verification of entanglement of the above class of states was demonstrated by using the approach based on the sum of mutual information. It can be checked that the above class of states is entangled for $p \neq 0$ by using the positive partial transpose criterion [66]. For this class of states, Negativity as defined in Ref. [48] can be calculated from the partial transposed density matrix is given by

$$\mathcal{N}(\rho_{cc}(p)) = (d-1)\frac{p}{2}. \quad (12)$$

Since the one-parameter family of states given by Eq. (11) is separable for $p = 0$ and for $p \neq 0$, $\mathcal{N}(\rho_{cc}(p)) > 0$, this class of states is entangled if and only if $p > 0$.

Let us now consider the colored-noise two-qutrit maximally entangled state, i.e., $\rho_{cc}(p)$ given by Eq. (11) with $d = 3$. Let the basis $\{|a_j\rangle\}$ of the pair of observables $A_1 B_1$ in Eq. (2) be the computational basis and the basis $\{|b_j\rangle\}$ of the pair of observables $A_2 B_2$ in Eq. (2) be the generalized σ_y basis. For this choice of two MUBs, the sum of two PCCs for the colored-noise two-qutrit maximally entangled state is given by

$$|C_{A_1 B_1}| + |C_{A_2 B_2}| = 1 + p > 1 \quad \text{iff } p > 0, \quad (13)$$

which implies that the above sum of two PCCs being greater than 1 provides a necessary and sufficient criterion for certification of entanglement of the colored-noise mixed with two-qutrit maximally entangled state since, as mentioned earlier, this class of mixed states is entangled if and only if $p \neq 0$. See Appendix B for the derivation of the above expression for the sum of two PCCs.

It is then readily seen from the expression of Negativity for the colored-noise two-qutrit maximally entangled state given by Eq. (12) with $d = 3$ that the sum of PCCs given by Eq. (13)

is related to Negativity as follows:

$$|C_{A_1 B_1}| + |C_{A_2 B_2}| = 1 + \mathcal{N}(\rho_{cc}(p)), \quad (14)$$

thereby providing quantification of entanglement in this case. On the other hand, it can be checked that for any two noncommuting bases which are *not* MUBs chosen from the set given by Eq. (6), the sum of two PCCs being greater than 1 provides *only* sufficient certification of entanglement of the colored-noise two-qutrit maximally entangled state.

Colored-noise mixed states-B. In addition to the above type of mixed state involving colored noise, we now consider the following type of state which was first introduced by Eltschka *et al.* in Ref. [56] and later used by Sentis *et al.* in Ref. [67].

Let us write as follows the general expression for this type of mixed state which is a mixture of the two-qudit maximally entangled state $|\phi_d^+\rangle$ and the colored-noise two-qudit state of the type given by $1/(d(d-1)) \sum_{i \neq j=0}^{d-1} |ij\rangle\langle ij|$:

$$\rho_{ac}(p) = p|\phi_d^+\rangle\langle\phi_d^+| + \frac{(1-p)}{d(d-1)} \sum_{i \neq j=0}^{d-1} |ij\rangle\langle ij|, \quad (15)$$

where $0 \leq p \leq 1$. For this class of states, Negativity as defined in Ref. [48] can be calculated from the partial transposed density matrix, given by

$$\mathcal{N}(\rho_{ac}(p)) = \max \left\{ \frac{dp-1}{2}, 0 \right\}. \quad (16)$$

Let us now consider the colored-noise two-qutrit maximally entangled state, i.e., $\rho_{ac}(p)$ given by Eq. (15) with $d = 3$. It can be checked that for the two MUBs which are the computational bases and the generalized σ_y basis, the sum of two PCCs for the colored-noise mixed states given by Eq. (15) with $d = 3$ is greater than 1 only when the Negativity is greater than certain value. Therefore, we proceed to check whether the sum of four PCCs for this family of mixed states is greater than 1 for some suitable set of four noncommuting bases if and only if the Negativity of the state is nonzero. We now use the set of four noncommuting bases (which are not MUBs) given in Eq. (6) which we have used for certifying and quantifying entanglement of the above mentioned two-qutrit isotropic state using the sum of four PCCs. For these noncommuting bases, the sum of four PCCs for the colored-noise two-qutrit mixed state given by Eq. (15) with $d = 3$ is given by

$$\sum_{i=1}^4 |C_{A_i B_i}| = \frac{9p-1}{2} > 1 \quad \text{iff } p > 1/3, \quad (17)$$

which implies that the above sum of two PCCs is greater than 1 if and only if the Negativity $\mathcal{N}(\rho_{ac}(p)) \neq 0$. See Appendix C for the derivation of the above expression for the sum of four PCCs. It is then readily seen from the expression of Negativity for the colored-noise two-qutrit maximally entangled state given by Eq. (16) with $d = 3$ that the sum of PCCs given by Eq. (17) is related to Negativity as

$$\sum_{i=1}^4 |C_{A_i B_i}| = 1 + 3\mathcal{N}(\rho_{ac}(p)), \quad (18)$$

thereby providing quantification of certified entanglement, similar to the quantification of entanglement of the two-qutrit isotropic states given by Eq. (10).

C. Werner states

In Ref. [57], Werner introduced a class of mixed two-qudit states for which there are separable as well as entangled subsets, the latter containing states for which local realist model exists. These mixed two-qudit states are called Werner states. Here we consider a particular form of such a state in any dimension which is a convex mixture of the projector onto the antisymmetric space and white noise [68] given by

$$\rho_W(p) = \frac{p}{d(d-1)} 2P_{\text{anti}} + \frac{(1-p)}{d^2} \mathbb{I}, \quad (19)$$

where

$$1 - \frac{2d}{d+1} \leq p \leq 1$$

and

$$P_{\text{anti}} = \frac{1}{2} \left(\mathbb{I} - \sum_{i,j=0}^{d-1} |i\rangle\langle j| \otimes |j\rangle\langle i| \right),$$

which is the projector onto the antisymmetric space. Note that for $d = 2$, the above class of states is a mixture of the maximally entangled state and white noise.

For the two-qudit Werner state $\rho_W(p)$ given by Eq. (19), Negativity as defined in Ref. [48] can be computed from the partial transposed density matrix and is given by

$$\mathcal{N}(\rho_W(p)) = \max \left\{ \frac{(d+1)p-1}{d^2}, 0 \right\}, \quad (20)$$

which is nonzero if and only if $p > 1/(d+1)$. Also, note that the two-qudit Werner state $\rho_W(p)$ given by Eq. (19) is entangled if and only if $p > 1/(d+1)$ [57,68]. Therefore, it follows that the Negativity of this class of states as given by Eq. (20) provides the necessary and sufficient quantification of entanglement for any d . We may note here that for $d \geq 3$, the existence of an entanglement witness for such class of states which is experimentally measurable has been shown [69] but the quantification of certified entanglement of the Werner states has remained uninvestigated. Thus, in this context, the following procedure of entanglement characterization using the measurable PCCs is of particular significance.

Let us now consider the two-qutrit Werner state, i.e., $\rho_W(p)$ given by Eq. (19) with $d = 3$. For the four noncommuting bases (which are not MUBs) given in Eq. (6), i.e., $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, and $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, the sum of four PCCs for the two-qutrit Werner state is given by

$$\sum_{i=1}^4 |C_{A_i B_i}| = 2|p| > 1 \quad \text{iff} \quad p > 1/2. \quad (21)$$

See Appendix D for the derivation of the above expression. Since, as mentioned earlier, the Werner states given by Eq. (19) with $d = 3$ are entangled for $p > 1/4$, it follows from Eq. (21) that the sum of four PCCs being greater than 1 provides a sufficient criterion for the certification of entanglement

of the state given by Eq. (20) with $d = 3$. Interestingly, it is found that the expression for the sum of four PCCs obtained in Eq. (21) for the two-qutrit Werner states can also be obtained by the set of four MUBs given by Eq. (E1) in Appendix E. Next, we argue that the sum of PCCs given by Eq. (21) also provides quantification of certified entanglement of the Werner states.

Note that using Eq. (20), Negativity of the two-qutrit Werner state for $p > 1/4$ given by

$$\mathcal{N}(\rho_W(p)) = \frac{4p-1}{9}. \quad (22)$$

From Eq. (22), using Eq. (21) it follows that for $p > 1/4$

$$\sum_{i=1}^4 |C_{A_i B_i}| = \frac{1 + 9\mathcal{N}(\rho_W(p))}{2}. \quad (23)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

D. Werner-Popescu states

The so-called Werner-Popescu state [52,55] in arbitrary dimension d which is a convex mixture of the maximally entangled pure two-qudit state and white noise is given by

$$\rho_{WP}(p) = \frac{1-p}{d^2} \mathbb{I} + p |\phi_d^+\rangle\langle\phi_d^+|, \quad (24)$$

which has also been discussed elsewhere, for instance, in Ref. [32]. For $d = 2$, Werner-Popescu states become same as the Werner states up to local unitary.

Note that the isotropic mixed state given by Eq. (3) can be written in the form of $\rho_{WP}(p)$ given above with $F = \frac{(d^2-1)p+1}{d^2}$, for $F \geq 1/d^2$ since p lies between 0 and 1. Now, $F > 1/d$ implies $p > 1/(d+1)$ and, as mentioned earlier, the two-qudit isotropic state is entangled if and only if $F > 1/d$. It thus follows that the two-qudit Werner-Popescu state $\rho_{WP}(p)$ given by Eq. (24) is entangled if and only if $p > 1/(d+1)$ [52].

Let us now consider the two-qutrit Werner-Popescu state, i.e., $\rho_{WP}(p)$ given by Eq. (24) with $d = 3$. For the choice of four noncommuting bases (not MUBs) given by Eq. (6), the sum of four PCCs for the two-qutrit Werner-Popescu state is given by

$$\sum_{i=1}^4 |C_{A_i B_i}| = 4p > 1 \quad \text{iff} \quad p > 1/4. \quad (25)$$

See Appendix G for the derivation of the above expression for the sum of four PCCs. Since, as mentioned earlier, the Werner-Popescu state given by Eq. (24) with $d = 3$ is entangled if and only if $p > 1/4$, the sum of four PCCs as given above being greater than 1 provides necessary and sufficient certification of entanglement.

While the above demonstration of necessary and sufficient certification of entanglement has been in terms of four noncommuting bases which are *not* MUBs, it can be checked that for the set of four MUBs which include the computational basis and generalized σ_x basis, the sum of four PCCs being greater than 1 provides *only* sufficient certification of entanglement of the two-qutrit Werner-Popescu states. Next,

we argue that the sum of PCCs given by Eq. (25) also provides quantification of certified entanglement of the two-qutrit Werner-Popescu states in the following sense.

For the two-qutrit Werner-Popescu state $\rho_{WP}(p)$ given by Eq. (24) with $d = 3$, Negativity as defined in Ref. [48] can be computed from the partial transposed density matrix and is given by

$$\mathcal{N}(\rho_{WP}(p)) = \max \left\{ \frac{4p-1}{3}, 0 \right\}, \quad (26)$$

which is nonzero if and only if $p > 1/4$. Interestingly, the two-qutrit isotropic mixed state $\rho_{WP}(p)$ is entangled if and only if $p > 1/4$ [52]. Therefore, it follows that the Negativity of this class of states as given by Eq. (26) provides the necessary and sufficient quantification of entanglement.

Now, note that using Eq. (26), one can write Negativity of the two-qutrit Werner-Popescu state $\rho_{WP}(p)$ for $p > 1/4$

$$\mathcal{N}(\rho_{WP}(p)) = \frac{4p-1}{3}. \quad (27)$$

From Eq. (27), using Eq. (25) it follows that for $p > 1/4$

$$\sum_{i=1}^4 |\mathcal{C}_{A_i B_i}| = 1 + 3\mathcal{N}(\rho_{WP}(p)). \quad (28)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

Next, we proceed to investigate to what extent the approach using PCCs can provide certification and quantification of entanglement for the pure states and the above classes of states for $d = 4$ and 5 as well as pure states.

III. TWO-QUIDIT STATES FOR $d = 4$ AND $d = 5$

A. Pure states

For $d = 4$. Let us consider the pure two-qudit state of dimension $d = 4$ of the form

$$|\psi_4\rangle = c_0 |00\rangle + c_1 |11\rangle + c_2 |22\rangle + c_3 |33\rangle, \quad (29)$$

where $0 \leq c_0, c_1, c_2, c_3 \leq 1$, and $\sum_{i=0}^3 c_i^2 = 1$. For the above class of states, the expression for Negativity is given by

$$\mathcal{N}(|\psi_4\rangle) = c_0 c_1 + c_0 c_2 + c_0 c_3 + c_1 c_2 + c_1 c_3 + c_2 c_3. \quad (30)$$

The above expression can be obtained from the general formula for Negativity for a pure two-qudit state $|\psi_d\rangle$ given by [56]

$$\mathcal{N}(|\psi_d\rangle) = \sum_{p \neq q=0, p)q}^{d-1} c_p c_q, \quad (31)$$

where $|\psi_d\rangle$ is of the Schmidt decomposition form

$$|\psi_d\rangle = \sum_{i=0}^{d-1} c_i |ii\rangle. \quad (32)$$

In Sec. II A, the generalized σ_z basis and the generalized σ_y basis have been defined for any dimension $d \geq 3$. For this choice of two MUBs in the case $d = 4$, the sum of two PCCs for the pure two-qudit states of dimension $d = 4$ given by

Eq. (29) can be shown to be given by

$$\begin{aligned} & |\mathcal{C}_{A_1 B_1}| + |\mathcal{C}_{A_2 B_2}| \\ &= 1 + \frac{9c_2 c_3 + c_1(9c_2 + 2c_3) + c_0(9c_1 + 2c_2 + 9c_3)}{10}, \end{aligned} \quad (33)$$

where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ and $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, with $\{|a_j\rangle\}$ and $\{|b_j\rangle\}$ being the generalized σ_z basis and the generalized σ_y basis, respectively, and the eigenvalues are given by $a_0 = b_0 = +2$, $a_1 = b_1 = +1$, $a_2 = b_2 = -1$, and $a_3 = b_3 = -2$. From Eqs. (30) and (33) it follows that if and only if any two of c_i 's are nonzero, then Negativity is nonzero as well as the sum of PCCs given by Eq. (33) is greater than 1. Now, since a pure two-qudit state is entangled if and only if Negativity is nonvanishing, we can argue that for the pure two-qudit states of dimension $d = 4$, the sum of PCCs being greater than 1 provides necessary and sufficient certification of entanglement. Note that the sum of PCCs given by Eq. (33) attains the algebraic maximum of 2 for the maximally entangled state for which all c_i s in Eq. (33) are equal to $1/\sqrt{4}$.

As regards quantification of entanglement, it can be checked that the sum of PCCs given by Eq. (33) is related to Negativity as

$$|\mathcal{C}_{A_0 B_0}| + |\mathcal{C}_{A_1 B_1}| = 1 + \frac{9\mathcal{N}(|\psi_4\rangle) - 7\chi}{10}, \quad (34)$$

where $\chi = c_0 c_2 + c_1 c_3$ which takes value in the interval $0 \leq \chi \leq 1/2$. The relationship between the sum of PCCs and Negativity given above implies that for any class of pure states for which the quantity χ takes a constant value c , the sum of PCCs given by Eq. (33) is a monotonic function of Negativity. This means that for any pair of pure states within a class of pure states for which $\chi = c$, a higher value of the sum of PCCs given by Eq. (34) always implies higher degree of entanglement.

For the more general class of pure states given by Eq. (29), whether the sum of PCCs for any other possible two MUBs is a monotonic function of Negativity is a critical issue.

For $d = 5$. Let us consider the general pure two-qudit state of dimension $d = 5$ given by

$$|\psi_5\rangle = c_0 |00\rangle + c_1 |11\rangle + c_2 |22\rangle + c_3 |33\rangle + c_4 |44\rangle, \quad (35)$$

where $0 \leq c_0, c_1, c_2, c_3, c_4 \leq 1$, and $\sum_{i=0}^4 c_i^2 = 1$. For the above class of states, the general expression for Negativity given by Eq. (31) reduces to

$$\begin{aligned} \mathcal{N}(|\psi_5\rangle) &= c_0(c_1 + c_2 + c_3 + c_4) + c_1(c_2 + c_3 + c_4) \\ &\quad + c_2(c_3 + c_4) + c_3 c_4. \end{aligned} \quad (36)$$

For the two MUBs which are taken to be the generalized σ_z basis and the generalized σ_y basis for $d = 5$, the sum of two PCCs for the pure two-qudit states of dimension $d = 5$ given by Eq. (35) can be shown to be given by

$$\begin{aligned} & |\mathcal{C}_{A_1 B_1}| + |\mathcal{C}_{A_2 B_2}| \\ &= 1 + \frac{5 + \sqrt{5}}{10} (c_0 c_1 + c_0 c_4 + c_1 c_2 + c_2 c_3 + c_3 c_4) \\ &\quad + \frac{5 - \sqrt{5}}{10} (c_0 c_2 + c_0 c_3 + c_1 c_3 + c_1 c_4 + c_2 c_4), \end{aligned} \quad (37)$$

where, similar to that mentioned for $d = 4$, we have taken $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ and $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, with $\{|a_j\rangle\}$ and $\{|b_j\rangle\}$ being the generalized σ_z basis and the generalized σ_y basis, respectively, and the eigenvalues are given by $a_0 = b_0 = +2$, $a_1 = b_1 = +1$, $a_2 = b_2 = 0$, $a_3 = b_3 = -1$, and $a_4 = b_4 = -2$. The above sum of PCCs given by Eq. (37) attains the algebraic maximum of 2 for the maximally entangled state for which all c_i s in Eq. (37) are equal to $1/\sqrt{5}$.

Now, from Eqs. (36) and (37) it follows that if and only if any two of c_i 's are nonzero, then Negativity is nonzero as well as the sum PCCs given by Eq. (33) is greater than 1. Thus, for the pure two-qudit states of dimension $d = 5$, the sum of PCCs being greater than 1 provides necessary and sufficient certification of entanglement.

As regards quantification of entanglement, it can be checked that the sum of PCCs given in Eq. (37) is related to the Negativity as

$$|C_{A_0B_0}| + |C_{A_1B_1}| = 1 + \frac{(5 + \sqrt{5})\mathcal{N}(|\psi_5\rangle) - 2\sqrt{5}\chi}{10}, \quad (38)$$

where $\chi = c_0c_2 + c_0c_3 + c_1c_3 + c_1c_4 + c_2c_4$ which takes value in the interval $0 \leq \chi \leq 1$. Similar to the case of $d = 4$ pure states, the relationship between the sum of PCCs and Negativity given above implies that for any pair of pure states drawn from a class of pure states for which the quantity χ takes a constant value c , a higher value of the sum of the PCCs given by Eq. (38) always implies higher value of entanglement.

B. Isotropic mixed states

Now, following the procedure of entanglement characterization using the measurable PCCs as shown for two-qutrit isotropic mixed states, we now proceed to address the $d = 4$ and $d = 5$ cases.

For $d = 4$. Now, to certify entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 4$, we use the sum of five PCCs $\sum_{i=1}^5 |C_{A_iB_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, and $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$ with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = -1$, and $a_3 = b_3 = e_3 = g_3 = k_3 = -2$. Detailed expressions for the five bases corresponding to these observables are given by Eq. (F1) in Appendix F. For this choice of five mutually unbiased bases, the sum of five PCCs is given by

$$\sum_{i=1}^5 |C_{A_iB_i}| = \frac{|16F - 1|}{3} > 1 \quad \text{iff } F > 1/4. \quad (39)$$

Since the isotropic mixed state [given by Eq. (3)] is entangled for $F > 1/4$ for dimension $d = 4$, it follows that the sum of five PCCs given by Eq. (39) being greater than 1 provides a necessary and sufficient criterion for the certification of entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 4$. Next, we argue that the sum of PCCs given by Eq. (39) also provides quantification of certified entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 4$.

Note that using Eq. (5), one can write Negativity of the entangled isotropic mixed state [given by Eq. (3)] in dimension $d = 4$ for $F > 1/4$ given by

$$\mathcal{N}(\rho_I(p)) = \frac{4F - 1}{2}. \quad (40)$$

From Eq. (40), using Eq. (39) it follows that for $F > 1/4$

$$\sum_{i=1}^5 |C_{A_iB_i}| = 1 + \frac{8}{3}\mathcal{N}(\rho_I(p)). \quad (41)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

For $d = 5$. Similarly, now, to certify entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 5$, we use the sum of six PCCs $\sum_{i=1}^6 |C_{A_iB_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$, and $A_6 = B_6 = \sum_j l_j |l_j\rangle\langle l_j|$ with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = l_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = l_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = l_2 = 0$, $a_3 = b_3 = e_3 = g_3 = k_3 = l_3 = -1$, and $a_4 = b_4 = e_4 = g_4 = k_4 = l_4 = -2$. Detailed expressions for the six bases corresponding to these observables are given by Eq. (F2) in Appendix F. For this choice of six noncommuting bases which are not MUBs, the sum of six PCCs is given by

$$\sum_{i=1}^6 |C_{A_iB_i}| = \frac{|25F - 1|}{4} > 1 \quad \text{iff } F > 1/5. \quad (42)$$

Since the isotropic mixed state given by Eq. (3) is entangled for $F > 1/5$ for dimension $d = 4$, it follows that the sum of six PCCs given by Eq. (42) being greater than 1 provides a necessary and sufficient criterion for the certification of entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 5$. Similar to the case $d = 4$, we now argue that the sum of PCCs given by Eq. (42) also provides quantification of certified entanglement of the isotropic mixed state given by Eq. (3) in dimension $d = 5$ in the following sense.

Now, note that using Eq. (5), one can write Negativity of the entangled isotropic mixed state [given by Eq. (3)] in dimension $d = 5$ for $p > 1/5$ given by

$$\mathcal{N}(\rho_I(F)) = \frac{5F - 1}{2}. \quad (43)$$

From Eq. (43), using Eq. (42) it follows that for $F > 1/5$

$$\sum_{i=1}^6 |C_{A_iB_i}| = 1 + \frac{5}{2}\mathcal{N}(\rho_I(F)). \quad (44)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

C. Colored-noise mixed with maximally entangled state

Here we consider two types of a colored-noise state mixed with the maximally entangled two-qudit state given by Eqs. (11) and (15) which are abbreviately called colored-noise mixed states-*A* and colored-noise mixed states-*B*, respectively.

1. Colored-noise mixed states-A

For $d = 4$. In order to certify entanglement of the colored-noise two-qudit maximally entangled state [given by Eq. (11)] in dimension $d = 4$ as in the case for $d = 3$, we use the criterion given by Eq. (2). Let the basis $\{|a_j\rangle\}$ of the pair of observables A_1B_1 in Eq. (2) be the computational basis and the basis $\{|b_j\rangle\}$ of the pair of observables A_2B_2 in Eq. (2) be the generalized σ_y basis. For this choice of two MUBs, the sum of two PCCs computed for the state given by Eq. (11) for $d = 4$ is given by

$$|C_{A_1B_1}| + |C_{A_2B_2}| = 1 + p > 1 \quad \text{iff } p > 0, \quad (45)$$

from which it follows that the above sum of two PCCs being greater than 1 provides a necessary and sufficient criterion for certification of entanglement of the colored-noise mixed with two-qudit maximally entangled state in dimension $d = 4$ since, as mentioned earlier, this class of mixed states is entangled if and only if $p \neq 0$. It is also readily seen from Eqs. (45) and (12) for $d = 4$ that the sum of PCCs is related to Negativity as follows:

$$|C_{A_1B_1}| + |C_{A_2B_2}| = 1 + \frac{2}{3}\mathcal{N}(\rho_{cc}(p)), \quad (46)$$

thereby providing quantification of entanglement in this case.

For $d = 5$. Similar to the above case, we consider the basis $\{|a_j\rangle\}$ of the pair of observables A_1B_1 in Eq. (2) to be the computational basis and the basis $\{|b_j\rangle\}$ of the pair of observables A_2B_2 in Eq. (2) to be the generalized σ_y basis. For this choice of two MUBs, the sum of two PCCs computed using the state given by Eq. (11) for $d = 5$ is given by

$$|C_{A_1B_1}| + |C_{A_2B_2}| = 1 + p > 1 \quad \text{iff } p > 0, \quad (47)$$

which shows, similar to the earlier case for $d = 4$, that the above sum of two PCCs being greater than 1 provides a necessary and sufficient criterion for certification of entanglement of the colored-noise mixed with two-qudit maximally entangled state in dimension $d = 5$. It is then also seen from Eqs. (47) and (12) for $d = 5$ that the sum of two PCCs is related to Negativity as follows:

$$|C_{A_1B_1}| + |C_{A_2B_2}| = 1 + \frac{1}{2}\mathcal{N}(\rho_{cc}(p)) > 1 \quad \text{iff } \mathcal{N} > 0, \quad (48)$$

thereby providing quantification of entanglement in this case.

2. Colored-noise mixed states-B

For $d = 4$. Now, to certify entanglement of the colored-noise mixed state given by Eq. (15) in dimension $d = 4$, we use the sum of five PCCs $\sum_{i=1}^5 |C_{A_iB_i}|$ for the five noncommuting bases given by Eq. (F1) in Appendix F which we have used in the case of entanglement certification of isotropic mixed states in $d = 4$. This sum of PCCs takes the following expression for the colored-noise mixed state given by Eq. (15) in dimension $d = 4$:

$$\sum_{i=1}^5 |C_{A_iB_i}| = \frac{|16p - 1|}{3} > 1 \quad \text{iff } p > 1/4. \quad (49)$$

The colored-noise mixed state [given by Eq. (15)] has Negativity for dimension $d = 4$ given by

$$\mathcal{N}(\rho_{ac}(p)) = \frac{4p - 1}{2}, \quad (50)$$

for $p \geq 1/4$ which implies that the sum of five PCCs given by Eq. (49) is greater than 1 if and only if the Negativity of the state is nonzero. Next, we argue that the sum of PCCs given by Eq. (50) also provides quantification of certified entanglement of the mixed state given by Eq. (15) in dimension $d = 4$. From Eq. (50), using Eq. (49) it follows that for $p > 1/4$

$$\sum_{i=1}^5 |C_{A_iB_i}| = 1 + \frac{8}{3}\mathcal{N}(\rho_{ac}(p)). \quad (51)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies certified entanglement.

For $d = 5$. Similarly, now, to certify entanglement of the colored-noise mixed state given by Eq. (15) in dimension $d = 5$, we use the sum of six PCCs $\sum_{i=1}^6 |C_{A_iB_i}|$ for the six noncommuting bases given by Eq. (F2) in Appendix F with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = l_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = l_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = l_2 = 0$, $a_3 = b_3 = e_3 = g_3 = k_3 = l_3 = -1$, and $a_4 = b_4 = e_4 = g_4 = k_4 = l_4 = -2$. This sum of six PCCs takes the following expression for the colored-noise mixed state given by Eq. (15) in $d = 5$:

$$\sum_{i=1}^6 |C_{A_iB_i}| = \frac{|25p - 1|}{4} > 1 \quad \text{iff } p > 1/5. \quad (52)$$

The colored-noise mixed state [given by Eq. (15)] has Negativity for dimension $d = 5$ given by

$$\mathcal{N}(\rho_{ac}(p)) = \frac{5p - 1}{2} \quad (53)$$

for $p \geq 1/5$, which implies that the sum of six PCCs given by Eq. (52) is greater than 1 if and only if the Negativity of the state is nonzero. Next, we argue that the sum of PCCs given by Eq. (53) also provides quantification of certified entanglement of the mixed state given by Eq. (15) in dimension $d = 5$. From Eq. (53), using Eq. (52) it follows that for $p > 1/5$

$$\sum_{i=1}^6 |C_{A_iB_i}| = 1 + \frac{5}{2}\mathcal{N}(\rho_{ac}(p)). \quad (54)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies certified entanglement.

D. Werner states

Now, following the procedure of entanglement characterization using the PCCs as shown for two-qutrit Werner states, we now proceed to address the $d = 4$ and $d = 5$ cases.

For $d = 4$. In order to certify entanglement of the Werner state given by Eq. (19) in dimension $d = 4$, we invoke the sum of five PCCs $\sum_{i=1}^5 |C_{A_iB_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, and $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$. Using the five noncommuting bases which are

MUBs given by Eq. (F1) in Appendix F with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = -1$, and $a_3 = b_3 = e_3 = g_3 = k_3 = -2$, the sum of five PCCs in this case computed for the state given by Eq. (19) for $d = 4$ is

$$\sum_{i=1}^5 |C_{A_i B_i}| = \frac{5}{3} |p| > 1 \quad \text{iff} \quad p > 3/5. \quad (55)$$

Since the Werner states given by Eq. (19) are entangled for $p > 1/5$ in dimension $d = 4$, it follows that the sum of five PCCs given by Eq. (55) being greater than 1 provides a sufficient criterion for the certification of entanglement of the Werner states in dimension $d = 4$. Next, we argue that the sum of PCCs given by Eq. (55) also provides quantification of certified entanglement of the Werner states in the following sense.

For the two-qudit Werner state $\rho_W(p)$ given by Eq. (19) in dimension $d = 4$, Negativity as defined in Ref. [48] computed from the partial transposed density matrix is given by

$$\mathcal{N}(\rho_W(p)) = \max \left\{ \frac{5p-1}{16}, 0 \right\}, \quad (56)$$

which is nonzero if and only if $p > 1/5$. Now, note that using Eq. (56), one can write for $p > 1/5$

$$\mathcal{N}(\rho_W(p)) = \frac{5p-1}{16}. \quad (57)$$

From Eq. (57), using Eq. (55) it follows that for $p > 1/5$

$$\sum_{i=1}^5 |C_{A_i B_i}| = \frac{1 + 16\mathcal{N}(\rho_W(p))}{3}. \quad (58)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement for the Werner state [Eq. (19)] for $d = 4$.

For $d = 5$. In order to certify entanglement of the Werner state given by Eq. (19) in dimension $d = 5$, we use the sum of six PCCs $\sum_{i=1}^6 |C_{A_i B_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, and $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$. For the six noncommuting bases (which are not MUBs) given by Eq. (F2) in Appendix F with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = -1$, and $a_3 = b_3 = e_3 = g_3 = k_3 = -2$, the sum of six PCCs is given as

$$\sum_{i=1}^6 |C_{A_i B_i}| = \frac{3}{2} |p| > 1 \quad \text{iff} \quad p > 2/3. \quad (59)$$

Since the Werner states given by Eq. (19) are entangled for $p > 1/6$ in dimension $d = 5$, it follows that the sum of six PCCs given by Eq. (59) being greater than 1 provides a sufficient criterion for the certification of entanglement of the Werner states given by Eq. (19) in dimension $d = 5$. Interestingly, it is found that the expression for the sum of six PCCs obtained in Eq. (59) can also be obtained by the set of six MUBs given by Eq. (E2) in Appendix E. Next, we

argue that the sum of PCCs given by Eq. (59) also provides quantification of certified entanglement of the Werner states.

For the two-qudit Werner state $\rho_W(p)$ given by Eq. (19) in dimension $d = 5$, Negativity as defined in Ref. [48] computed from the partial transposed density matrix is given by

$$\mathcal{N}(\rho_W(p)) = \max \left\{ \frac{6p-1}{25}, 0 \right\}, \quad (60)$$

which is nonzero if and only if $p > 1/6$. Now, note that using Eq. (60), one can write for $p > 1/6$

$$\mathcal{N}(\rho_W(p)) = \frac{6p-1}{25}. \quad (61)$$

From Eq. (61), using Eq. (59) it follows that for $p > 1/6$

$$\sum_{i=1}^6 |C_{A_i B_i}| = \frac{1 + 25\mathcal{N}(\rho_W(p))}{4}. \quad (62)$$

Thus the sum of PCCs is a linear function of Negativity and hence quantifies entanglement for the Werner state [Eq. (19)] for $d = 5$.

E. Werner-Popescu states

Here we address the entanglement characterization of the two-qudit Werner-Popescu states in the $d = 4$ and $d = 5$ cases using PCCs, similar to the way discussed for the two-qudit Werner-Popescu states.

For $d = 4$. Now, to certify entanglement of the Werner-Popescu state given by Eq. (24) in dimension $d = 4$, we use the sum of five PCCs $\sum_{i=1}^5 |C_{A_i B_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$ and $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$. For the choice of five mutually unbiased bases given by Eq. (F1) in Appendix F with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = -1$, and $a_3 = b_3 = e_3 = g_3 = k_3 = -2$, the sum of five PCCs is given by

$$\sum_{i=1}^5 |C_{A_i B_i}| = 5p > 1 \quad \text{iff} \quad p > 1/5. \quad (63)$$

Since the Werner-Popescu state [given by Eq. (24)] is entangled for $p > 1/5$ for dimension $d = 4$, it follows that the sum of five PCCs given by Eq. (63) being greater than 1 provides a necessary and sufficient criterion for the certification of entanglement of the Werner-Popescu state given by Eq. (24) in dimension $d = 4$. Next, we argue that the sum of PCCs given by Eq. (63) also provides quantification of certified entanglement of the Werner-Popescu state given by Eq. (24) in dimension $d = 4$.

For the Werner-Popescu state [given by Eq. (24)] in $d = 4$, Negativity as defined in Ref. [48] can be computed from the partial transposed density matrix and is given by

$$\mathcal{N}(\rho_{WP}(p)) = \max \left\{ \frac{3(5p-1)}{8}, 0 \right\}, \quad (64)$$

which is nonzero if and only if $p > 1/5$. Therefore, it follows that Negativity of the Werner-Popescu state given by Eq. (24) in $d = 4$ provides the necessary and sufficient quantification

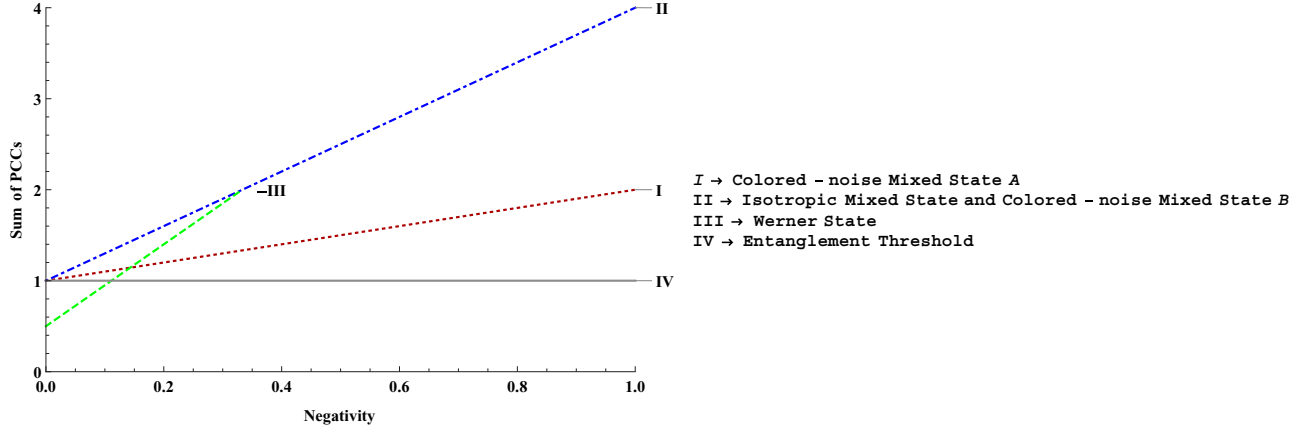


FIG. 2. For $d = 3$, the sum of PCCs is plotted as a function of Negativity for the six families of two-qudit states indicated in the right-hand side. The dotted line (I) corresponds to the sum of two PCCs versus Negativity for the colored-noise mixed state A given by Eq. (13). The dot-dashed line (II) denotes the sum of four PCCs versus Negativity for the isotropic mixed state, colored-noise mixed state B and Werner-Popescu state given by Eqs. (8), (17), and (25), respectively. The dashed line (III) indicates the sum of four PCCs versus Negativity for the Werner states given by Eq. (23). The horizontal line (IV) specifies entanglement threshold above which the states are entangled.

of entanglement. Note that using Eq. (64), one can write Negativity of the entangled isotropic mixed state in $d = 4$ as

$$\mathcal{N}(\rho_{WP}(p)) = \frac{3(5p-1)}{8}. \quad (65)$$

From Eq. (65), using Eq. (63) it follows that for $p > 1/5$

$$\sum_{i=1}^5 |C_{A_i B_i}| = 1 + \frac{8}{3} \mathcal{N}(\rho_{WP}(p)). \quad (66)$$

Hence the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case.

For $d = 5$. Similarly, now, to certify entanglement of the Werner-Popescu state given by Eq. (24) in dimension $d = 5$, we use the sum of six PCCs $\sum_{i=1}^6 |C_{A_i B_i}|$, where $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$, $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, $A_5 = B_5 = \sum_j k_j |k_j\rangle\langle k_j|$ and $A_6 = B_6 = \sum_j l_j |l_j\rangle\langle l_j|$. For the choice of six noncommuting bases which are not MUBs given by Eq. (F2) in Appendix F with the eigenvalues $a_0 = b_0 = e_0 = g_0 = k_0 = l_0 = +2$, $a_1 = b_1 = e_1 = g_1 = k_1 = l_1 = +1$, $a_2 = b_2 = e_2 = g_2 = k_2 = l_2 = 0$, $a_3 = b_3 = e_3 = g_3 = k_3 = l_3 = -1$, and $a_4 = b_4 = e_4 = g_4 = k_4 = l_4 = -2$, the sum of six PCCs is given by

$$\sum_{i=1}^6 |C_{A_i B_i}| = 6p > 1 \quad \text{iff} \quad p > 1/6. \quad (67)$$

Since the generalized Werner-Popescu state given by given by Eq. (24) is entangled for $p > 1/6$ for dimension $d = 5$, it follows that the sum of six PCCs given by Eq. (67) being greater than 1 provides a necessary and sufficient criterion for the certification of entanglement of the isotropic mixed state (24) in dimension $d = 5$. Similar to the case $d = 4$, we now argue that the sum of PCCs given by Eq. (67) also provides quantification of certified entanglement of the generalized Werner-Popescu state (24) in dimension $d = 5$ in the following sense.

For the Werner-Popescu state [given by Eq. (24)] in $d = 5$, Negativity as defined in Ref. [48] is given by

$$\mathcal{N}(\rho_{WP}(p)) = \max \left\{ \frac{2(6p-1)}{5}, 0 \right\}, \quad (68)$$

which is nonzero if and only if $p > 1/6$. Therefore, Negativity of the Werner-Popescu state in $d = 5$ provides the necessary and sufficient quantification of entanglement. Now, using Eq. (68), Negativity of the entangled Werner-Popescu state in $d = 5$ is given by

$$\mathcal{N}(\rho_{WP}(p)) = \frac{2(6p-1)}{5}. \quad (69)$$

Using Eq. (67) it then follows that for $p > 1/6$

$$\sum_{i=1}^6 |C_{A_i B_i}| = 1 + \frac{5}{2} \mathcal{N}(\rho_{WP}(p)). \quad (70)$$

Thus, the sum of PCCs is a linear function of Negativity and hence quantifies entanglement in this case, too.

Note that Negativity of the Werner-Popescu state does not have a closed form of expression for arbitrary dimension d as in the case of isotropic state. Nevertheless, it is interesting that the relationship between the sum of $d + 1$ PCCs and Negativity for the two-qudit Werner-Popescu state in the cases of $d = 3, 4$, and 5 given by Eqs. (28), (66), and (70), respectively, has the same form as that for the two-qudit isotropic state in these cases given by Eqs. (10), (41), and (44), respectively.

IV. CONCLUDING REMARKS

In a nutshell, the work reported here demonstrates for dimensions $d = 3, 4$, and 5 that the scheme formulated here relating the experimentally measurable Pearson correlation coefficients (PCCs) with Negativity as an entanglement measure is able to provide necessary and sufficient certification as well as quantification of entanglement for a range of physically relevant mixed states such as isotropic states, colored-noise mixed states-A and Werner-Popescu states (see Figs. 2–4

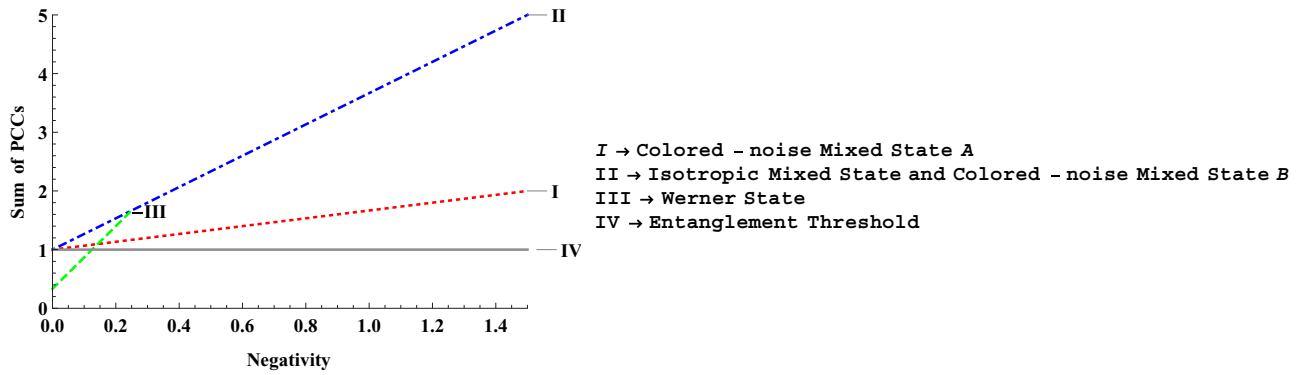


FIG. 3. For $d = 4$, the sum of PCCs is plotted as a function of Negativity for the six families of two-qudit states indicated in the right-hand side. The dotted line (I) corresponds to the sum of two PCCs versus Negativity for the colored-noise mixed state A given by Eq. (46). The dot-dashed line (II) denotes the sum of five PCCs versus Negativity for the isotropic mixed state, colored-noise mixed state B and Werner-Popescu state given by Eqs. (41), (51), and (63), respectively. The dashed line (III) indicates the sum of five PCCs versus Negativity for the Werner states given by Eq. (58). The horizontal line (IV) specifies entanglement threshold above which the states are entangled.

illustrating the results). Even for the Werner states in higher dimensions whose entanglement characterization has remained less explored by other approaches, the scheme discussed here in terms of PCCs is shown to furnish sufficient certification along with quantification of entanglement for dimensions $d = 3, 4$, and 5 (also shown in Figs. 2–4). Comparing the sufficient certification of entanglement for the Werner states using the PCC-based approach with that provided by the entanglement certification procedure [69] based on $d + 1$ mutually unbiased measurements, an interesting feature is noted that the range of values of the mixedness parameter for which the Werner states for $d = 3, 4$, and 5 are, respectively, certified to be entangled by both the approaches turn out to be the same (see Table I). However, the quantification of entanglement in these cases has remained unanalyzed in terms of the other approach [69], while in our paper the PCC-based approach is shown to be able to quantify entanglement of the Werner states for $d = 3, 4$, and 5 . Further, for the colored-noise mixed states-B, we show that PCCs can be used for quantification of certified entanglement when Negativity is nonvanishing. Thus, the range of results obtained in this paper

serve to reveal the strength of the PCC-based approach and provides impetus for investigating its extension for entanglement characterization in even higher dimensions than what has been considered in this work.

A key revelation of our treatment is that, among different measures of entanglement in high dimensions, it is Negativity as the measure of entanglement which is found to be analytically and monotonically related to the quantitative measure of correlations using combinations of PCCs in noncommuting bases (which may or may not be mutually unbiased). On the other hand, for pure states in any dimension, it has been argued that it is the correlation in mutually unbiased bases as quantified by a suitable information-theoretic measure which is directly related to the entanglement of formation [70,71]. The physical meaning of the latter as entanglement measure for the higher dimensional systems, interestingly, contrasts with that of Negativity. While entanglement of formation signifies the minimum number of “ebits” required to prepare a given state using local operations and classical communication [72,73], Negativity, as mentioned earlier [51], can be regarded as an estimator of how many degrees of freedom of

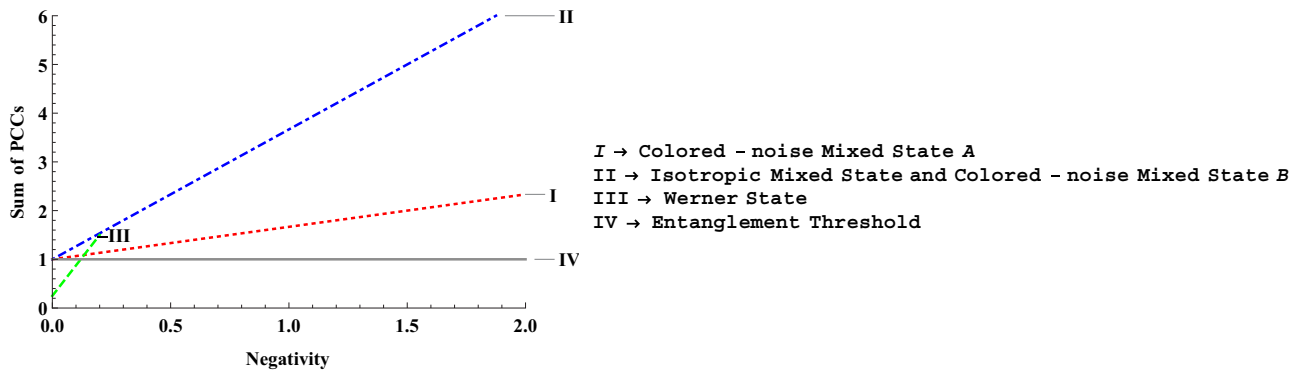


FIG. 4. For $d = 5$, the sum of PCCs is plotted as a function of Negativity for the six families of two-qudit states indicated in the right-hand side. The dotted line (I) corresponds to the sum of two PCCs versus Negativity for the colored-noise mixed state A given by Eq. (48). The dot-dashed line (II) denotes the sum of six PCCs versus Negativity for the isotropic mixed state, colored-noise mixed state B, and Werner-Popescu state given by Eqs. (44), (54), and (67), respectively. The dashed line (III) indicates the sum of six PCCs versus Negativity for the Werner states given by Eq. (62). The horizontal line (IV) specifies entanglement threshold above which the states are entangled.

TABLE I. The parameter ranges in which the Werner states for dimensions $d = 3, 4$, and 5 are, respectively, entangled are given in the first row. The second and third rows show, respectively, the parameter ranges in which the entanglement of Werner states in $d = 3, 4$, and 5 are certified, respectively, using the PCC-based approach and by invoking mutually unbiased measurements [69].

	Werner state in $d = 3$	Werner state in $d = 4$	Werner state in $d = 5$
Range of entanglement	$p > \frac{1}{4}$	$p > \frac{1}{5}$	$p > \frac{1}{6}$
Entanglement certification by $d + 1$ PCCs with noncommuting/MU bases	$p > \frac{1}{2}$	$p > \frac{3}{5}$	$p > \frac{2}{3}$
Entanglement certification based on $d + 1$ mutually unbiased measurements [69]	$p > \frac{1}{2}$	$p > \frac{3}{5}$	$p > \frac{2}{3}$

the subsystems are entangled, or, as determining the minimum number of dimensions involved in the quantum correlation. These notions, thus, require a deeper holistic probing by taking into account the various theoretical studies on different entanglement measures [74–80] and the comparison between Negativity and entanglement of formation experimentally studied for the first time for higher dimensional system in the accompanying paper [41].

Regarding the issue of physical implication of measures in terms of PCCs, it may be stressed that PCC is essentially a normalized covariance and covariance of measurement results is a natural measure of correlations widely used in diverse areas of science. Results presented in this paper showing that the sum of PCCs exceeding the classical bound certifies entanglement, highlights that quantum correlations underlying entanglement are stronger than corresponding classical correlations. Interestingly, even Bell-type local realist inequality has been formulated in terms of PCCs, which is extendable to two-qutrit states [39]. Thus, PCCs can be used not only for entanglement certification and quantification as discussed in this paper, but also for demonstrating nonlocality for two-qubit and two-qutrit states. Hence Pearson correlators could be key ingredients for empirically probing the quantitative relationship between entanglement and nonlocality. On the other hand, a PCC-based measure can also be useful for studying entanglement of distillation since PCCs are related to Negativity which, in turn, is related to the upper bound of entanglement of distillation [81].

Finally, it is important to note that our treatment has been restricted to NPT states. Thus, the extent to which the PCC-based approach for certifying entanglement would be applicable for PPT entangled (nondistillable) states is an open question. Our preliminary study using certain specific examples of two-qutrit bound entangled states indicates the following features: (a) For all the two-qutrit states belonging to the one parameter family of Horodecki bound entangled states [82], it is found that the sum of PCCs for the set of four noncommuting bases specified by Eq. (6) is always less than 1, thereby showing inapplicability of the PCC-based entanglement certification scheme for such states. (b) On the other hand, it is found that for both the two-qutrit bound entangled states [83,84] which show nonlocality through the violation of a suitable Bell-type inequality, the sum of PCCs for the set of four MUBs specified by Eq. (E1) with a different choice of eigenvalues and for the set of four noncommuting bases specified by Eq. (6) with a different choice of eigenvalues, respectively, is greater than 1, thereby certifying entanglement for such states. These results, therefore, underscore the need for a comprehensive study of the extent of applicability of the

PCC-based approach for the entanglement characterisation of bound entangled states.

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APPENDIX A: DERIVATION OF EQ. (8) FOR THE SUM OF FOUR PCCs FOR THE TWO-QUTRIT ISOTROPIC MIXED STATES

For $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ in which the basis $\{|a_j\rangle\}$ is the computational basis and the eigenvalues a_j are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, calculating the relevant single and joint expectation values of the two-qutrit isotropic states given by Eq. (5) with $d = 3$, it can be checked that the PCC in this case takes the value

$$C_{A_1 B_1} = \frac{-1 + 9p}{8}. \quad (\text{A1})$$

For $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, where the basis $\{|b_j\rangle\}$ is given in Eq. (6) and the eigenvalues b_j are given by $b_0 = 0$, $b_1 = \pm 1$, and $b_2 = \mp 1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_2 B_2} = \frac{1 - 9p}{8}. \quad (\text{A2})$$

For $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, where the basis $\{|e_j\rangle\}$ is given in Eq. (6) and the eigenvalues e_j are given by $e_0 = +1$, $e_1 = 0$, and $e_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case takes the value

$$C_{A_3 B_3} = \frac{1 - 9p}{8}. \quad (\text{A3})$$

For $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, where the basis $\{|g_j\rangle\}$ is given in Eq. (6) and the eigenvalues g_j are given by $g_0 = +1$, $g_1 = 0$, and $g_2 = -1$, calculating the relevant single and joint expectation values, the PCC in this case is given by

$$C_{A_4 B_4} = \frac{1 - 9p}{8}. \quad (\text{A4})$$

Then Eq. (8) follows from Eqs. (A1)–(A4).

APPENDIX B: DERIVATION OF EQ. (13) FOR THE SUM OF TWO PCCs FOR THE COLORED-NOISE TWO-QUTRIT MAXIMALLY ENTANGLED STATE-A

For $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ in which the basis $\{|a_j\rangle\}$ is the computational basis and the eigenvalues a_j are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, the relevant single and joint expectation values for the colored-noise two-qutrit maximally entangled state given by Eq. (11) with $d = 3$, it can be checked that the PCC in this case takes the value

$$C_{A_1 B_1} = 1. \quad (\text{B1})$$

For $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$ in which the basis $\{|b_j\rangle\}$ is the generalized σ_y basis and the eigenvalues b_j are given by $b_0 = +1$, $b_1 = 0$, and $b_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_2 B_2} = -p. \quad (\text{B2})$$

Then Eq. (13) follows from Eqs. (B1) and (B2).

APPENDIX C: DERIVATION OF EQ. (17) FOR THE SUM OF FOUR PCCs FOR THE COLORED-NOISE TWO-QUTRIT MAXIMALLY ENTANGLED STATE-B

For $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ in which the basis $\{|a_j\rangle\}$ is the computational basis and the eigenvalues a_j are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, the relevant single and joint expectation values of the colored-noise two-qutrit maximally entangled state given by Eq. (15) with $d = 3$, it can be checked that the PCC in this case takes the value

$$C_{A_1 B_1} = \frac{-1 + 3p}{2}. \quad (\text{C1})$$

For $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, where the basis $\{|b_j\rangle\}$ is given in Eq. (6) and the eigenvalues b_j are given by $b_0 = 0$, $b_1 = \pm 1$, and $b_2 = \mp 1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_2 B_2} = -p. \quad (\text{C2})$$

For $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, where the basis $\{|e_j\rangle\}$ is given in Eq. (6) and the eigenvalues e_j are given by $e_0 = +1$, $e_1 = 0$, and $e_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case takes the value

$$C_{A_3 B_3} = -p. \quad (\text{C3})$$

For $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, where the basis $\{|g_j\rangle\}$ is given in Eq. (6) and the eigenvalues g_j are given by $g_0 = +1$, $g_1 = 0$, and $g_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_4 B_4} = -p. \quad (\text{C4})$$

Then Eq. (17) follows from Eqs. (C1)–(C4).

APPENDIX D: DERIVATION OF EQ. (21) FOR THE SUM OF PCCs FOR THE TWO-QUTRIT WERNER STATES

For $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ in which the basis $\{|a_j\rangle\}$ is the computational basis and the eigenvalues a_j are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, the relevant single and joint expectations of the two-qutrit Werner states given by Eq. (19) with $d = 3$, it can be checked that the PCC in this case takes the value

$$C_{A_1 B_1} = \frac{-P}{2}. \quad (\text{D1})$$

For $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, where the basis $\{|b_j\rangle\}$ is given in Eq. (6) and the eigenvalues b_j are given by $b_0 = 0$, $b_1 = \pm 1$, and $b_2 = \mp 1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_2 B_2} = \frac{-P}{2}. \quad (\text{D2})$$

For $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, where the basis $\{|e_j\rangle\}$ is given in Eq. (6) and the eigenvalues e_j are given by $e_0 = +1$, $e_1 = 0$, and $e_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case takes the value

$$C_{A_3 B_3} = \frac{-P}{2}. \quad (\text{D3})$$

For $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, where the basis $\{|g_j\rangle\}$ is given in Eq. (6) and the eigenvalues g_j are given by $g_0 = +1$, $g_1 = 0$, and $g_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_4 B_4} = \frac{-P}{2}. \quad (\text{D4})$$

Then Eq. (21) follows from Eqs. (D1)–(D4).

APPENDIX E: $d + 1$ MUTUALLY UNBIASED BASES WHICH CAN BE USED FOR CERTIFYING ENTANGLEMENT OF $d = 3$ AND 5 WERNER STATES

To obtain the expression for the sum of four PCCs given in Eq. (21) for the two-qutrit Werner states, one can also use the following four mutually unbiased bases:

$$\begin{aligned} \{|a_j\rangle\} &= \{|0\rangle, |1\rangle, |2\rangle\}, \\ \{|b_j\rangle\} &= \{(|0\rangle + \omega |1\rangle + \omega^2 |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + |1\rangle + |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega |2\rangle)/\sqrt{3}\}, \\ \{|e_j\rangle\} &= \{(|0\rangle + \omega |1\rangle + \omega |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + |1\rangle + \omega^2 |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + |2\rangle)/\sqrt{3}\}, \\ \{|g_j\rangle\} &= \{(|0\rangle + \omega^2 |1\rangle + \omega^2 |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + |1\rangle + \omega |2\rangle)/\sqrt{3}, \\ &\quad (|0\rangle + \omega |1\rangle + |2\rangle)/\sqrt{3}\}, \end{aligned} \quad (\text{E1})$$

where $\omega = e^{2i\pi/3}$.

The expression obtained for the sum of six PCCs in Eq. (21) for the Werner states in $d = 5$ can also be obtained by using the following six mutually unbiased bases:

$$\begin{aligned} \{|a_j\rangle\} &= \{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle\}, \\ \{|b_j\rangle\} &= \{(|0\rangle + \omega^3 |1\rangle + \omega |2\rangle + \omega^4 |3\rangle + \omega^2 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + \omega^3 |2\rangle + \omega^2 |3\rangle + \omega |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + |1\rangle + |2\rangle + |3\rangle + |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega |1\rangle + \omega^2 |2\rangle + \omega^3 |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega^4 |2\rangle + \omega |3\rangle + \omega^3 |4\rangle)/\sqrt{5}\}, \\ \{|e_j\rangle\} &= \{(|0\rangle + \omega^3 |1\rangle + \omega^3 |2\rangle + |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + |2\rangle + \omega^3 |3\rangle + \omega^3 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + |1\rangle + \omega^2 |2\rangle + \omega |3\rangle + \omega^2 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega |1\rangle + \omega^4 |2\rangle + \omega^4 |3\rangle + \omega |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega |2\rangle + \omega^2 |3\rangle + |4\rangle)/\sqrt{5}\}, \\ \{|g_j\rangle\} &= \{(|0\rangle + \omega^4 |1\rangle + \omega^2 |2\rangle + \omega^4 |3\rangle + |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + |1\rangle + \omega^4 |2\rangle + \omega^2 |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega |1\rangle + \omega |2\rangle + |3\rangle + \omega^3 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega^3 |2\rangle + \omega^3 |3\rangle + \omega^2 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + |2\rangle + \omega |3\rangle + \omega |4\rangle)/\sqrt{5}\}, \\ \{|k_j\rangle\} &= \{(|0\rangle + |1\rangle + \omega |2\rangle + \omega^4 |3\rangle + \omega |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega |1\rangle + \omega^4 |2\rangle + \omega |3\rangle + |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + |2\rangle + \omega^4 |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + \omega^2 |2\rangle + \omega^2 |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + \omega^4 |2\rangle + |3\rangle + \omega^2 |4\rangle)/\sqrt{5}\}, \\ \{|l_j\rangle\} &= \{(|0\rangle + \omega |1\rangle + |2\rangle + \omega^2 |3\rangle + \omega^2 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega^2 |2\rangle + |3\rangle + \omega |4\rangle)/\sqrt{5}, \end{aligned}$$

$$\begin{aligned} &(|0\rangle + \omega^3 |1\rangle + \omega^4 |2\rangle + \omega^4 |3\rangle + |4\rangle)/\sqrt{5}, \\ &(|0\rangle + \omega^4 |1\rangle + \omega |2\rangle + \omega |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &(|0\rangle + |1\rangle + \omega^3 |2\rangle + \omega^4 |3\rangle + \omega^3 |4\rangle)/\sqrt{5}\}, \quad (E2) \end{aligned}$$

where $\omega = 2i\pi/5$.

APPENDIX F: $d + 1$ NONCOMMUTING BASES USED FOR CALCULATING THE SUM OF $d + 1$ PCCs IN THE CASE OF $d = 4$ AND 5 ISOTROPIC AND WERNER STATES

For calculating the sum of five PCCs in the case of $d = 4$ isotropic states and Werner states, we consider the following choice of five mutually unbiased bases:

$$\begin{aligned} \{|a_j\rangle\} &= \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}, \\ \{|b_j\rangle\} &= \{(|0\rangle + |1\rangle + |2\rangle + |3\rangle)/2, \\ &\quad (|0\rangle + |1\rangle - |2\rangle - |3\rangle)/2, \\ &\quad (|0\rangle - |1\rangle - |2\rangle + |3\rangle)/2, \\ &\quad (|0\rangle - |1\rangle + |2\rangle - |3\rangle)/2\}, \\ \{|e_j\rangle\} &= \{(|0\rangle + |1\rangle + i |2\rangle - i |3\rangle)/2, \\ &\quad (|0\rangle - |1\rangle + i |2\rangle + i |3\rangle)/2, \\ &\quad (|0\rangle - |1\rangle - i |2\rangle - i |3\rangle)/2, \\ &\quad (|0\rangle + |1\rangle - i |2\rangle + i |3\rangle)/2\}, \\ \{|g_j\rangle\} &= \{(|0\rangle - i |1\rangle - |2\rangle - i |3\rangle)/2, \\ &\quad (|0\rangle + i |1\rangle + |2\rangle - i |3\rangle)/2, \\ &\quad (|0\rangle - i |1\rangle + |2\rangle + i |3\rangle)/2, \\ &\quad (|0\rangle + i |1\rangle - |2\rangle + i |3\rangle)/2\}, \\ \{|k_j\rangle\} &= \{(|0\rangle + i |1\rangle - i |2\rangle + |3\rangle)/2, \\ &\quad (|0\rangle - i |1\rangle + i |2\rangle + |3\rangle)/2, \\ &\quad (|0\rangle + i |1\rangle + i |2\rangle - |3\rangle)/2, \\ &\quad (|0\rangle - i |1\rangle - i |2\rangle - |3\rangle)/2\}. \quad (F1) \end{aligned}$$

Now, for calculating the sum of six PCCs in the case of $d = 5$ isotropic states and Werner states, we consider the following choice of six noncommuting bases:

$$\begin{aligned} \{|a_j\rangle\} &= \{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle\}, \\ \{|b_j\rangle\} &= \{(|0\rangle + \omega^3 |1\rangle + \omega |2\rangle + \omega^4 |3\rangle + \omega^2 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^4 |1\rangle + \omega^3 |2\rangle + \omega^2 |3\rangle + \omega |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + |1\rangle + |2\rangle + |3\rangle + |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega |1\rangle + \omega^2 |2\rangle + \omega^3 |3\rangle + \omega^4 |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 |1\rangle + \omega^4 |2\rangle + \omega |3\rangle + \omega^3 |4\rangle)/\sqrt{5}\}, \\ \{|e_j\rangle\} &= \{(|0\rangle + e^{i\pi/5} |1\rangle + e^{2i\pi/5} |2\rangle + e^{3i\pi/5} |3\rangle + e^{4i\pi/5} |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega e^{i\pi/5} |1\rangle + \omega^2 e^{2i\pi/5} |2\rangle + \omega^3 e^{3i\pi/5} |3\rangle + \omega^4 e^{4i\pi/5} |4\rangle)/\sqrt{5}, \\ &\quad (|0\rangle + \omega^2 e^{i\pi/5} |1\rangle + \omega^4 e^{2i\pi/5} |2\rangle + \omega e^{3i\pi/5} |3\rangle + \omega^3 e^{4i\pi/5} |4\rangle)/\sqrt{5}, \end{aligned}$$

$$\begin{aligned}
 & (|0\rangle + \omega^3 e^{i\pi/5} |1\rangle + \omega e^{2i\pi/5} |2\rangle + \omega^4 e^{3i\pi/5} |3\rangle + \omega^2 e^{4i\pi/5} |4\rangle)/\sqrt{5}, \\
 & (|0\rangle + \omega^4 e^{i\pi/5} |1\rangle + \omega^3 e^{2i\pi/5} |2\rangle + \omega^2 e^{3i\pi/5} |3\rangle + \omega e^{4i\pi/5} |4\rangle)/\sqrt{5}, \\
 \{|g_j\rangle\} = & \{(\omega^2 |0\rangle + \omega^3 |1\rangle + \omega |2\rangle + \omega^4 |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega |0\rangle + \omega^4 |1\rangle + \omega^3 |2\rangle + \omega^2 |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (|0\rangle + |1\rangle + |2\rangle + |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega^4 |0\rangle + \omega |1\rangle + \omega^2 |2\rangle + \omega^3 |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega^3 |0\rangle + \omega^2 |1\rangle + \omega^4 |2\rangle + \omega |3\rangle + |4\rangle)/\sqrt{5}\}, \\
 \{|k_j\rangle\} = & \{(e^{4i\pi/5} |0\rangle + e^{i\pi/5} |1\rangle + e^{2i\pi/5} |2\rangle + e^{3i\pi/5} |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega^4 e^{4i\pi/5} |0\rangle + \omega e^{i\pi/5} |1\rangle + \omega^2 e^{2i\pi/5} |2\rangle + \omega^3 e^{3i\pi/5} |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega^3 e^{4i\pi/5} |0\rangle + \omega^2 e^{i\pi/5} |1\rangle + \omega^4 e^{2i\pi/5} |2\rangle + \omega e^{3i\pi/5} |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega^2 e^{4i\pi/5} |0\rangle + \omega^3 e^{i\pi/5} |1\rangle + \omega e^{2i\pi/5} |2\rangle + \omega^4 e^{3i\pi/5} |3\rangle + |4\rangle)/\sqrt{5}, \\
 & (\omega e^{4i\pi/5} |0\rangle + \omega^4 e^{i\pi/5} |1\rangle + \omega^3 e^{2i\pi/5} |2\rangle + \omega^2 e^{3i\pi/5} |3\rangle + |4\rangle)/\sqrt{5}\}, \\
 \{|l_j\rangle\} = & \{(\omega^3 |0\rangle + \omega |1\rangle + \omega^4 |2\rangle + \omega^2 |3\rangle - |4\rangle)/\sqrt{5}, \\
 & (\omega^4 |0\rangle + \omega^3 |1\rangle + \omega^2 |2\rangle + \omega |3\rangle - |4\rangle)/\sqrt{5}, \\
 & (|0\rangle + |1\rangle + |2\rangle + |3\rangle - |4\rangle)/\sqrt{5}, \\
 & (\omega |0\rangle + \omega^2 |1\rangle + \omega^3 |2\rangle + \omega^4 |3\rangle - |4\rangle)/\sqrt{5}, \\
 & (\omega^2 |0\rangle + \omega^4 |1\rangle + \omega |2\rangle + \omega^3 |3\rangle - |4\rangle)/\sqrt{5}\}, \tag{F2}
 \end{aligned}$$

where $\omega = 2i\pi/5$. It can be checked that the above noncommuting bases are *not* unbiased to each other.

APPENDIX G: DERIVATION OF EQ. (25) FOR THE SUM OF FOUR PCCs FOR THE TWO-QUTRIT WERNER-POPESCU STATES

For $A_1 = B_1 = \sum_j a_j |a_j\rangle\langle a_j|$ in which the basis $\{|a_j\rangle\}$ is the computational basis and the eigenvalues a_j are given by $a_0 = +1$, $a_1 = 0$, and $a_2 = -1$, the relevant single and joint expectation values of the two-qutrit Werner-Popescu states given by Eq. (24) with $d = 3$, it can be checked that the PCC in this case takes the value

$$C_{A_1 B_1} = p. \tag{G1}$$

For $A_2 = B_2 = \sum_j b_j |b_j\rangle\langle b_j|$, where the basis $\{|b_j\rangle\}$ is given in Eq. (6) and the eigenvalues b_j are given by $b_0 = 0$, $b_1 = \pm 1$, and $b_2 = \mp 1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in

this case is given by

$$C_{A_2 B_2} = -p. \tag{G2}$$

For $A_3 = B_3 = \sum_j e_j |e_j\rangle\langle e_j|$, where the basis $\{|e_j\rangle\}$ is given in Eq. (6) and the eigenvalues e_j are given by $e_0 = +1$, $e_1 = 0$, and $e_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case takes the value

$$C_{A_3 B_3} = -p. \tag{G3}$$

For $A_4 = B_4 = \sum_j g_j |g_j\rangle\langle g_j|$, where the basis $\{|g_j\rangle\}$ is given in Eq. (6) and the eigenvalues g_j are given by $g_0 = +1$, $g_1 = 0$, and $g_2 = -1$, calculating the relevant single and joint expectation values, it can be checked that the PCC in this case is given by

$$C_{A_4 B_4} = -p. \tag{G4}$$

Then Eq. (25) follows from Eqs. (G1)–(G4).

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