Self-testing of multiple unsharpness parameters through sequential violations of a noncontextual inequality

Rajdeep Paul,[1,*] Souradeep Sasmal ,[2,1,†] and A. K. Pan [1,‡]

[1]*Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana 502285, India*

[2]*Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 611731, China*

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Self-testing protocols refer to novel device-independent certification schemes wherein the devices are uncharacterized and the dimension of the system remains unspecified. The optimal quantum violation of Bell's inequality facilitates such self-testing. In this work we put forth a protocol for self-testing of noisy quantum instruments, specifically, the unsharpness parameter of smeared projective measurements in any arbitrary dimension. Our protocol hinges on the sequential quantum violations of a bipartite Bell-type preparation noncontextual inequality, involving three measurement settings per party. First, we demonstrate that at most three sequential independent Bobs manifest simultaneous preparation contextuality with a single Alice through the violation of this inequality. Subsequently, we show that the suboptimal sequential quantum violations of the noncontextual inequality form an optimal set, eventually enabling the self-testing of a shared state, local measurements, and unsharpness parameters of one party. Notably, we derive the optimal set of quantum violations without specifying the dimension of the quantum system, thereby circumventing the constraint that may arise due to Naimark's theorem. Furthermore, we extend our investigation to quantify the degree of incompatible measurements pertaining to the sequential observers, exploring how variations in the degree of incompatibility impact the values of unsharp parameters necessary for sequential quantum violation.

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I. INTRODUCTION

Self-testing represents a novel approach that facilitates the strongest possible form of device-independent (DI) certification of quantum systems solely from the observed input-output statistics [1]. In such a protocol, quantum devices are considered to be black boxes and the dimension of the quantum system is unknown. The DI self-testing relies on the optimal quantum violation of a suitable Bell inequality [2], enabling unique characterization of the state and measurements. For instance, the optimal violation of the Clauser-Horn-Shimony-Holt (CHSH) inequality [3] self-tests the bipartite state to be maximally entangled, and local observables are anticommuting [4]. Besides a plethora of applications in information-theoretic tasks, the DI self-testing provides foundational insights into understanding the geometric structure of the set of quantum correlations. It is worth noting that the optimal quantum violation of a Bell inequality signifies that the quantum correlation in question is an extremal point of the set of all quantum correlations.

Since the inception of the self-testing protocol by Mayers and Yao [5], a flurry of protocols have been proposed, including parallel self-testing of multiple maximally entangled two-qubit states [6,7] and self-testing of the pure nonmaximally entangled two-qubit state [8–13]. Recent developments have extended self-testing protocols to multipartite scenarios. Using specific linear and quadratic Bell inequalities, self-testing of the N-partite Greenberger-Horne-Zeilinger state and anticommuting observables for each party has been demonstrated [14]. Additionally, self-testing of the tripartite W state has been proposed, utilizing the SWAP circuit method [15]. Moreover, self-testing protocols have been extended to higher-dimensional states, such as maximally entangled two-qudit states [16], as well as to multipartite graph states [17] and optimal states for XOR games [18]. Self-testing of measurements and inputs has been reported in [19,20]. Quite a number of works on self-testing of the nonprojective measurements in device-independent or semi-device-independent scenarios have used either the dimension of the quantum system or the prepare-and-measure scenario [19,21–25]. Recently, device-independent certification of an unsharp instrument was also reported [4]. The state and measurements have been self-tested in the experiment scenario in [26].

Note that the Bell inequality is a test of a notion of classicality widely known as local realism. A distinct perspective on classicality emerged through the work of Kochen and Specker [27] and later was generalized by Spekkens [28], who framed the notion of classicality in terms of noncontextuality. In this regard, recent developments support [29,30] that noncontextuality may constitute a more fundamental notion of classicality than that of local realism. This assertion is underpinned by establishing the connection between steering with preparation noncontextuality via measurement incompatibility and hence concluding noncontextual realist models as

*Contact author: ph21resch11016@iith.ac.in
†Contact author: souradeep.007@gmail.com
‡Contact author: akp@phy.iith.ac.in

a subset of local realist models [29–31]. This implies that even when a quantum correlation has an underlying local realist model, it may manifest nonclassicality in the form of contextuality. Apart from the immense foundational significance the nonlocality and contextuality pose, the latter, much like nonlocal correlations [1,32], emerges as a pivotal resource with diverse applications in the realm of information processing such as communication games [25,33–35], state discrimination [36–38], semi-device-independent randomness certification [39], sequential sharing of correlations [40], self-testing protocols [41,42], and quantum computation [43–45].

In this paper we aim to self-test noisy quantum instruments, specifically the unsharp parameter of the smeared version of projective measurement, through the sequential quantum violations of a preparation noncontextual inequality. Note that the unsharp measurement in a standard Bell experiment produces suboptimal quantum violation and hence any kind of certification becomes challenging. The suboptimal quantum violation in an experiment may arise from various factors, such as (i) the nonideal preparation of a state other than that which is intended, (ii) the inappropriate implementation of local observables, or (iii) the presence of noise in implementing projective measurements, which can be modeled as unsharp measurements [46,47]. Hence, the self-test of an unsharp quantum instrument inevitably requires the simultaneous DI certification of the state, observables, and unsharpness parameter from the same observed input-output statistics. Note that the effect of the unsharp measurements is reflected in the postmeasurement states and the standard Bell test is incapable of certifying them. We invoke sequential Bell experiments which have the potential to self-test the unsharpness parameter along with the state and measurements as the sequential quantum violations depend on the postmeasurement states. However, such sequential quantum violations are suboptimal and the challenge is to certify the state, measurements, and unsharpness parameter from a set of suboptimal quantum violations. Note that the sequential sharing of various forms of quantum correlation by multiple sequential observers has been extensively explored [40,48–51]. Our work can then be viewed as a potential application of such studies.

A Bell test involves two distant parties Alice and Bob who share a bipartite entangled state $\rho_1 \in \mathscr{H}^d \otimes \mathscr{H}^d$, where d is the dimension of the local system. A sequential Bell experiment involves a single Alice (who always performs sharp projective measurements of her two observables) and an arbitrary k numbers of sequential Bobs (say, Bob^k) who performs unsharp measurements. The kth Bob may perform sharp measurement. After performing unsharp measurements on their respective subsystems, Bob^1 passes his residual subsystem to another sequential observer Bob^2 and so forth. The process continues until Alice and Bob^k get the violation of Bell's inequality. The choice of unsharp measurement is imperative as projective measurements maximally disturb the system, thereby destroying the entanglement and hence sequential Bobs have no chance to get the violation of Bell's inequality.

To this end, it is worth noting here that recently, semi-DI certification of an unsharp instrument has been demonstrated both theoretically [23,42,52–57] and experimentally [58,59] by assuming a qubit system. Following this, quantification of the degree of incompatibility of two sequential pairs of quantum measurements has been demonstrated through the sequential quantum advantage [58]. The first DI certification of an unsharp instrument was proposed [4] based on the CHSH inequality [3].

In this work we demonstrate how suboptimal quantum violations form an optimal pair (or tuple) to self-test the unsharpness parameters of Bob^1. It was believed that the DI self-testing of the unsharp parameter is not possible due to Naimark's theorem, which states that any nonprojective measurement can be interpreted as the projective measurement in higher-dimensional space. Since in the DI scenario no dimension restriction is imposed, a stubborn individual always argues that the measurement is projective, but the experimentalist could not prepare the ideal observables required for the optimal quantum value. We overcome this by considering the dimension-independent optimization of sequential Bell values simultaneously. We invoke an elegant sum-of-square (SOS) approach to evaluate the suboptimal quantum value of the Bell functional in the sequential scenario, without assuming the dimension of the system. We demonstrate that a maximum of three independent sequential observers (Bob_1, Bob_2, and Bob_3) can demonstrate the suboptimal quantum violation of the inequality with a single Alice. This enables us to robustly certify the unsharpness parameters of Bob_1 and Bob_2.

Note that incompatible measurements are necessary to demonstrate the preparation contextual quantum correlations [29,30]. By quantifying the degree of incompatibility pertaining to Bob's observables, we establish a quantitative relationship between the degree of incompatibility and the sequential quantum violations of Bell's inequality. We note that such a relationship was introduced in [58], where the authors demonstrated how the degree of incompatibility for each pair of Bob's measurements leads to sequential suboptimal violations of the CHSH inequality. However, they [58] considered the qubit system for their demonstration. We first show that such a relationship can be demonstrated without assuming the dimension of the quantum system. The sequential quantum violations of Bell's inequality certify unsharp parameters, enabling the certification of the degree of incompatibilities of each sequential Bob's observables. Further, we extend the analysis to trine observables based on the sequential quantum violations of our noncontextual inequality. By using the degree of incompatibility for three observables defined in [60,61], we quantitatively demonstrate how the degree of incompatibility for each sequential Bob can be certified from the suboptimal violations of the noncontextual inequality. We conclude with a summary and a brief discussion of future possibilities.

II. BELL FUNCTIONAL AND ITS PREPARATION NONCONTEXTUAL BOUND

We provide a brief overview of the ontological model of operational quantum theory and the notion of classicality in terms of noncontextuality. We consider a Bell functional whose upper bound in a preparation noncontextual model is lower than the local bound.

A. Ontological model and preparation noncontextuality

The primitives of an operational theory are a set of preparation procedures denoted by $\{\mathbb{P}\}$ and a set of measurement procedures denoted by $\{\mathbb{M}\}$. The probability of obtaining a specific outcome k is given by $p(k|\mathcal{P}, \mathcal{M})$. In operational quantum theory, a specific preparation procedure $\mathcal{P} \in \mathbb{P}$ prepares the quantum state ρ and the measurements $\mathcal{M} \in \mathbb{M}$ performed on the quantum state are in general characterized by a set of positive-semidefinite operators, known as positive-operator-valued measures (POVMs), denoted by $\{\mathcal{E}_k\}$, satisfying $\sum_k \mathcal{E}_k = \mathbb{1}$. The quantum probability is obtained from the Born rule, $p(k|\mathcal{M}, \rho) = \text{Tr}[\rho\mathcal{E}_k]$.

In an ontological model of quantum theory the preparation of ρ through a specific procedure yields an ontic state $\lambda \in \Lambda$ with a probability distribution $\mu(\lambda|\mathcal{P})$ satisfying $\sum_\Lambda \mu(\lambda|\mathcal{P}) = 1$, where Λ denotes the ontic state space. The probability of obtaining an outcome k is given by a response function $\mathscr{E}(k|\lambda, \mathcal{E}_k)$, with $\sum_k \mathscr{E}(k|\lambda, \mathcal{E}_k) = 1\,\forall\,\lambda$. Any ontological model that is consistent with quantum theory must reproduce the Born rule, i.e.,

$$\sum_\Lambda \mu(\lambda|\rho, \mathcal{P})\mathscr{E}(k|\lambda, \mathcal{M}) = \text{Tr}[\rho\mathcal{E}_k].$$

An ontological model of the operational theory is said to be preparation noncontextual [28] if two preparation procedures $\mathcal{P}_1$ and $\mathcal{P}_2$ yield the same quantum state ρ that cannot be operationally distinguished by any measurement, i.e.,

$$p(k|\mathcal{P}_1, \mathcal{M}) = p(k|\mathcal{P}_2, \mathcal{M}) \Rightarrow \mu(\lambda|\rho, \mathcal{P}_1) = \mu(\lambda|\rho, \mathcal{P}_2)\,\forall\,\lambda.$$

This means that in a preparation noncontextual ontic model, ontic state distributions are equivalent, irrespective of the preparation procedures.

B. Bipartite Bell functional for three inputs per party

We consider a Bell experiment featuring two spatially separated parties Alice and Bob. Alice (Bob) randomly performs one of three dichotomic local measurements $A_x \in \{A_1, A_2, A_3\}$ ($B_y \in \{B_1, B_2, B_3\}$). The respective measurement outcomes are denoted by $a, b \in \{+1, -1\}$. Given the above Bell scenario, consider the Bell functional

$$\mathcal{I} = (A_1 + A_2 - A_3) \otimes B_1 + (A_1 - A_2 + A_3) \otimes B_2 + (-A_1 + A_2 + A_3) \otimes B_3. \quad (1)$$

The quantum value of this Bell functional is given by $\mathscr{I} = \text{Tr}[\mathcal{I}\rho]$. In an ontological model, the local bound of the Bell functional is $\mathcal{I}_l \leqslant 5$ [62]. Note that while by employing a particular type of communication game referred to as parity oblivious communication game it has been shown [25] that the preparation noncontextual bound is $\mathcal{I}_{\text{PNC}} \leqslant 4$, here we revisit the evaluation of preparation noncontextual bound without invoking such a game.

Before proceeding further, let us briefly recapitulate the notion of preparation noncontextuality in the CHSH scenario [3] where Alice (Bob) measures two observables A_1 and A_2 (B_1 and B_2). Alice's two measurements on her local part of the shared state ρ_{AB} yield two density matrices on Bob's wing denoted by ρ_{A_1} and ρ_{A_2}. Naturally, $\rho_{A_1} = \rho_{A_2} \equiv \sigma$; otherwise the no-signaling condition will be violated. Such a feature can be assumed to be equivalent to that represented in an ontological model, if one assumes that the ontological model is preparation noncontextual, i.e., $\mu(\lambda|\sigma, A_1) = \mu(\lambda|\sigma, A_2)$. It is then intuitively straightforward to conclude that a quantum violation of the CHSH inequality can also be regarded as proof of preparation contextuality. As demonstrated in [63], in the CHSH scenario, preparation noncontextuality implies the locality assumption. A modified version of this proof is outlined in [4].

For the CHSH scenario, by using Bayes' theorem, the joint probability distribution in the ontological model can be expressed as [4,29]

$$p(a, b|A_x, B_y) = \sum_\lambda p(a|A_x, B_y)p(\lambda|a, A_x)p(b|B_y, \lambda). \quad (2)$$

Now the locality condition implies the marginal probability of Alice's side is independent of Bob's choice of observables and hence we can write

$$p(a, b|A_x, B_y) = \sum_\lambda p(a|A_x)p(\lambda|a, A_x)p(b|B_y, \lambda). \quad (3)$$

From Bayes' theorem, it follows that $p(a|A_x)p(\lambda|a, A_x) = \mu(\lambda|A_x)p(a|\lambda, A_x)$, where we specifically denote the probability distribution $p(\lambda|A_x)$ by $\mu(\lambda|A_x)$. Substituting this into Eq. (3), we get

$$p(a, b|A_x, B_y) = \sum_\lambda \mu(\lambda|A_x)p(a|\lambda, A_x)p(b|B_y, \lambda). \quad (4)$$

Assuming the preparation noncontextual for Bob's preparation by Alice, i.e., $\mu(\lambda|\rho, A_1) = \mu(\lambda|\rho, A_2) \equiv \mu(\lambda)$, we simplify Eq. (4) to

$$p(a, b|A_x, B_y) = \sum_\lambda \mu(\lambda)p(a|\lambda, A_x)p(b|B_y, \lambda). \quad (5)$$

This result aligns with the desired factorizability condition commonly derived for a local hidden-variable model. Therefore, we argue that whenever the joint probability distribution $p(a, b|A_x, B_y)$ in the ontological model satisfies the assumption of preparation noncontextuality, it inherently satisfies the locality condition in the ontological model.

Moving beyond the CHSH scenario, we introduce a nontrivial form of preparation noncontextuality in a Bell experiment involving more than two inputs. This involves imposing an additional relational constraint on Alice's measurement observables, expressed by the condition

$$\sum_x P(a, b|A_x, B_y) = \sum_x P(a \oplus 1, b|A_x, B_y)\,\forall\,b, y. \quad (6)$$

In quantum theory, when Alice and Bob share an entangled state ρ_{AB}, the above condition translates to

$$\sum_x \rho^a_{A_x} = \sum_x \rho^{a\oplus 1}_{A_x} \equiv \sigma. \quad (7)$$

Here $\rho^a_{A_x} = \text{Tr}_A(\rho_{AB}\Pi^a_{A_x} \otimes \mathbb{1})$ and Eq. (7) implies $A_1 + A_2 + A_3 = 0$. This introduces a nontrivial constraint on Alice's preparation procedures, leading to a local bound reduced to the preparation noncontextual bound $\mathcal{I}_{\text{PNC}} \leqslant 4$.

Thus, nontrivial preparation contextuality provides a weaker notion of nonlocality. It is important to note that the set of observables of Alice for which the optimal quantum value

$\mathscr{I}_{\text{opt}} = 6$ is achieved satisfies the condition given by Eq. (6). More precisely, our demonstration reveals that attaining the optimal quantum value $\mathscr{I}_{\text{opt}} = 6$ necessitates the fulfillment of the constraint $A_1 + A_2 + A_3 = 0$.

III. OPTIMAL QUANTUM BOUND OF THE BELL FUNCTIONAL $\mathcal{I}$

We derive the optimal quantum value of the Bell functional, given by Eq. (1), devoid of assuming the dimension of the quantum system and by utilizing an elegant SOS approach introduced in [64]. For this, we consider a positive-semidefinite operator γ, which can be expressed as $\gamma = \beta \mathbb{1}_d - \mathcal{I}$, where β is a positive real number and $\mathbb{1}_d$ is the identity operator in an arbitrary d-dimensional system. This can be proven by considering a set of operators L_y, which are linear functions of the observables (Hermitian operators) A_x and B_y, such that

$$\gamma = \frac{1}{2}\sum_{y=1}^{3} \omega_y L_y^\dagger L_y. \tag{8}$$

The operators L_y are defined as

$$L_y = \mathscr{A}_y \otimes \mathbb{1} - \mathbb{1} \otimes B_y \,\forall\, y \in [1, 3], \tag{9}$$

where $\mathscr{A}_y$ and ω_y are defined as

$$\mathscr{A}_1 = \frac{A_1 + A_2 - A_3}{\omega_1}, \quad \mathscr{A}_2 = \frac{A_1 - A_2 + A_3}{\omega_2},$$
$$\mathscr{A}_3 = \frac{-A_1 + A_2 + A_3}{\omega_3}, \quad \omega_y = \|\mathscr{A}_y\|_\rho, \tag{10}$$

where $\|\cdot\|$ is the Frobenius norm, given by $\|\mathcal{O}\| = \sqrt{\text{Tr}[\mathcal{O}^\dagger \mathcal{O} \rho]}$ and $\mathscr{I} = \text{Tr}[\mathcal{I}\rho]$. Now putting Eqs. (9) and (10) into Eq. (8) and noting that $A_x^\dagger A_x = B_y^\dagger B_y = \mathbb{1}_d$, we obtain

$$\text{Tr}[\gamma\rho] = -\mathscr{I} + \sum_{y=1}^{3} \omega_y. \tag{11}$$

Therefore, it follows from Eq. (11) that the quantum optimal value of $\mathcal{I}$ is attained when $\langle\gamma\rangle = \text{Tr}[\gamma\rho] = 0$, which in turn provides

$$\mathscr{I}_{\text{opt}} = \max\left(\sum_{y=1}^{3} \omega_y\right). \tag{12}$$

Evaluating ω_y from Eq. (10), we arrive at the relations

$$\omega_1 = \sqrt{3 + \langle\{A_1, A_2 - A_3\}\rangle_\rho - \langle\{A_2, A_3\}\rangle_\rho},$$
$$\omega_2 = \sqrt{3 + \langle\{A_1, -A_2 + A_3\}\rangle_\rho - \langle\{A_2, A_3\}\rangle_\rho},$$
$$\omega_3 = \sqrt{3 - \langle\{A_1, A_2 + A_3\}\rangle_\rho + \langle\{A_2, A_3\}\rangle_\rho}. \tag{13}$$

Next, using the convex inequality $\sum_{i=1}^{n} \omega_i \leqslant \sqrt{n \sum_{i=1}^{n} (\omega_i)^2}$, from Eqs. (12) and (13) we get

$$\begin{aligned}\mathscr{I}_{opt} &= \max \sqrt{3(\omega_1^2 + \omega_2^2 + \omega_3^2)} \\ &= \max \sqrt{3[12 - (A_1 + A_2 + A_3)(A_1 + A_2 + A_3)^\dagger]} \\ &= 6.\end{aligned} \tag{14}$$

Clearly, the optimal value occurs when $A_1 + A_2 + A_3 = 0$, implying $\omega_1 = \omega_2 = \omega_3 = 2$. It is straightforward to check that $A_1 + A_2 + A_3 = 0$ implies $\text{Tr}[\{A_x, A_{x'}\}\rho] = -1 \,\forall\, x \neq x' \in \{1, 2, 3\}$ and consequently $\text{Tr}[\{\mathscr{A}_y, \mathscr{A}_{y'}\}\rho] = -1 \,\forall\, y \neq y' \in \{1, 2, 3\}$.

State and observables for achieving optimal violation

The optimality condition $\text{Tr}[\gamma\rho] = 0 \,\forall\, \rho$ implies that $\sum_{y=1}^{3} \text{Tr}[L_y^\dagger L_y \ \rho] = 0 \,\forall\, \rho$. Given that $L_y^\dagger L_y$ are positive and Hermitian operators, this relation leads us to the crucial deduction that $\text{Tr}[L_y \rho] = 0 \,\forall\, y$. Hence, Eq. (9) allows us to express

$$\text{Tr}[L_y\rho] = 0 \Rightarrow \text{Tr}[\mathbb{1} \otimes B_y \rho] = \text{Tr}[\mathscr{A}_y \otimes \mathbb{1}\rho]. \tag{15}$$

Furthermore, to achieve optimal quantum violation, it is crucial for Alice's observable to satisfy the condition $\langle\{A_x, A_{x'}\}_{x\neq x'}\rangle_\rho = -1 \,\forall\, \rho$. As a consequence, $\langle\{\mathscr{A}_y, \mathscr{A}_{y'}\}_{y\neq y'}\rangle_\rho = -1 \,\forall\, \rho$. Therefore, based on Eq. (15), Bob's observable must satisfy $\langle\{B_y, B_{y'}\}_{y\neq y'}\rangle_\rho = -1 \,\forall\, \rho$ for optimal violation.

Since the optimality condition is $\text{Tr}[L_y^\dagger L_y \rho] = 0$, Eq. (9) leads to the inference that $\text{Tr}[\mathscr{A}_y \otimes B_y \rho] = 1 \,\forall\, y$. Thus, ρ must be a common eigenstate of the operators $\mathscr{A}_y \otimes B_y$ with $y = 1, 2, 3$. As these operators yield the maximum eigenvalue with the normalized state ρ, we can deduce that the state ρ is pure. As a result, we can expand ρ in terms of mutually commuting elements. However, since $[(\mathscr{A}_y \otimes B_y), (\mathscr{A}_{y'} \otimes B_{y'})]_{y\neq y'} \neq 0$, we are unable to express ρ in terms of $\mathscr{A}_y \otimes B_y$ in contrast to the CHSH scenario [see Eq. (7) of [4]].

Let us first consider the general form of ρ in the bipartite two-qubit scenario [65]

$$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{3} r_i \sigma_i \otimes \mathbb{1} + \sum_{j=1}^{3} s_j \mathbb{1} \otimes \sigma_j + \sum_{i,j=1}^{3} t_{ij} \sigma_i \otimes \sigma_j\right), \tag{16}$$

where $t_{ij} = \text{Tr}[\sigma_i \otimes \sigma_j \rho]$ are the elements of the correlation matrix $T = [t_{ij}]$ and r_i and s_j are positive real numbers, satisfying the relations [65]

$$\sum_{i=1}^{3} r_i^2 + \sum_{j=1}^{3} s_j^2 + \sum_{i,j=1}^{3} t_{ij}^2 \leqslant 3, \tag{17}$$

where the equality holds for pure states. Now let us consider that there exist a two-qubit state ρ and a set of Hermitian operators $\{C_i \neq \mathbb{1}\} \,\forall\, i \in \{1, 2, 3\}$ such that the condition $\text{Tr}[C_i \otimes C_i \rho] = 1$ holds. Then it is evident that $t_{ij} = 0 \,\forall\, i \neq j$ and $t_{ij} = \pm 1 \,\forall\, i = j$, implying $\sum_{i,j=1}^{3} t_{ij}^2 = 3$. Consequently, from Eq. (17) it follows that $\sum_{i=1}^{3} r_i^2 = \sum_{j=1}^{3} s_j^2 = 0$.

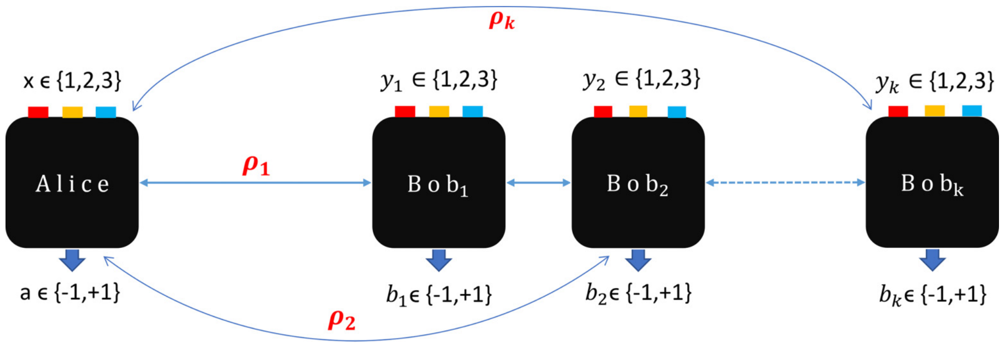

FIG. 1. Diagram depicting the sequential Bell scenario. Alice and Bob^1 share an entangled state $\rho_1 \in \mathscr{H}^d \otimes \mathscr{H}^d$. Alice always performs projective measurements and Bob^k performs unbiased unsharp POVMs.

Therefore, for the condition $\text{Tr}[C_i \otimes C_i \rho] = 1$ to be satisfied, the bipartite qubit state must be of the form

$$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{3} C_i \otimes C_i\right), \tag{18}$$

where $C_i \otimes C_i = t_{ii}\sigma_i \otimes \sigma_i$, satisfying $[C_i \otimes C_i, C_j \otimes C_j]_{i \neq j} = 0$. It is important to emphasize here that the state expressed by Eq. (18) is an entangled state, meeting the criterion $\text{Tr}_A(\rho) = \text{Tr}_B(\rho) = \frac{\mathbb{1}}{2}$ and $\rho^2 = \rho$. This signifies that ρ is a pure maximally entangled two-qubit state. The significant insight gained here is that a maximally entangled state can be represented in terms of mutually commuting operators.

Expanding on this notion, if we extend the idea to express a maximally entangled state in any arbitrary dimension d, we can represent ρ in terms of mutually commuting operators $C_i \otimes C_i$, which are functions of both $\mathscr{A}_y$ and B_y. Thus, ρ takes the form

$$\rho = \frac{1}{d^2}\left(\mathbb{1}_d \otimes \mathbb{1}_d + \sum_{i=1}^{d^2-1} C_i \otimes C_i\right). \tag{19}$$

Now, any three $C_i \otimes C_i$ can be derived based on the following optimality conditions obtained from the SOS approach: (i) $\text{Tr}[\mathscr{A}_y \otimes B_y \rho] = 1$, (ii) $\text{Tr}[C_i \otimes C_i \rho] = 1$, and (iii) $[C_i \otimes C_i, C_j \otimes C_j]_{i \neq j} = 0$. Using such conditions, we obtain the expressions for any three $C_i \otimes C_i$ (see Appendix A for detailed derivations),

$$\begin{aligned}
C_1 \otimes C_1 &= \mathscr{A}_1 \otimes B_1,\\
C_2 \otimes C_2 &= \tfrac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_3 \otimes B_2 - \mathscr{A}_2 \otimes B_3),\\
C_3 \otimes C_3 &= \tfrac{1}{3}(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1\\
&\quad + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1),
\end{aligned} \tag{20}$$

where $C_3 \otimes C_3$ satisfies the condition $C_3 \otimes C_3 = (C_2 \otimes C_2)(C_1 \otimes C_1)$. An explicit example for two-qubit maximally entangled state is

$$\rho = \tfrac{1}{4}(\mathbb{1} \otimes \mathbb{1} + \sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z). \tag{21}$$

If we compare the given form of ρ with the form given by Eq. (19), we can suitably choose $C_1 \otimes C_1 = \sigma_x \otimes \sigma_x$, $C_2 \otimes C_2 = \sigma_z \otimes \sigma_z$, and $C_3 \otimes C_3 = -\sigma_y \otimes \sigma_y$. Then, using Eqs. (10) and (20), we determine the following particular set of observables that leads to the optimal quantum violation:

$$\begin{aligned}
A_1 &= -B_3 = \frac{\sigma_x + \sqrt{3}\sigma_z}{2}, \quad A_2 = -B_2 = \frac{\sigma_x - \sqrt{3}\sigma_z}{2},\\
A_3 &= -B_1 = -\sigma_x.
\end{aligned} \tag{22}$$

IV. SEQUENTIAL QUANTUM VIOLATIONS OF NONCONTEXTUAL INEQUALITY

Let us quickly overview the sequential Bell experiment scenario [48]. Unlike the traditional Bell scenario with spatially separated Alice and Bob, we have one Alice who is spatially separated from multiple Bobs (see Fig. 1). Initially, a bipartite entangled state $\rho_1 \in \mathscr{H}^d \otimes \mathscr{H}^d$ is shared between Alice and Bob^1. Following the reception of their respective subsystems, Alice performs a projective measurement and Bob^1 performs unsharp measurements (unbiased POVM). Then Bob^1 passes his residual subsystem to the next sequential independent observer Bob^2. This process continues, with Bob^2 relaying his measured subsystem to Bob^3 and so forth.

The observables of Alice and Bob^k are given by

$$\begin{aligned}
A_x &\equiv \left\{A_{\pm|x} \mid A_{\pm|x} = \frac{1}{2}(\mathbb{1} \pm A_x)\right\} \forall x \in \{1, 2, 3\},\\
\mathcal{B}_y^k &= \left\{\mathcal{E}_{\pm|y}^k \mid \mathcal{E}_{\pm|y}^k = \frac{1}{2}(\mathbb{1} \pm \eta_k B_y^k)\right\} \forall y \in \{1, 2, 3\},
\end{aligned} \tag{23}$$

where $\mathcal{E}_{\pm|y}^k$ are POVM elements of Bob^k's measurement, satisfying $\mathcal{E}_{\pm|y}^k \geqslant 0$ and $\mathcal{E}_{+|y}^k + \mathcal{E}_{-|y}^k = \mathbb{1}$. The postmeasurement state ρ_k after the $(k-1)$th Bob's measurement is evaluated [66] as

$$\begin{aligned}
\rho_k &= \frac{1}{3}\sum_{y=1}^{3}\sum_{b=\pm}\left(\mathbb{1} \otimes \sqrt{B_{b|y}^{(k-1)}}\right)\rho_{AB^{k-1}}\left(\mathbb{1} \otimes \sqrt{B_{b|y}^{(k-1)}}\right)\\
&= \frac{1}{3}\sum_{b,y}\left[\left(\mathbb{1} \otimes \mathcal{K}_{b|y}^{k-1}\right)\rho_{k-1}\left(\mathbb{1} \otimes \mathcal{K}_{b|y}^{k-1}\right)\right]\\
&= \frac{1+\xi_{k-1}}{2}\rho_{k-1}\\
&\quad + \frac{1-\xi_{k-1}}{6}\sum_{y=1}^{3}\left(\mathbb{1} \otimes B_y^{k-1}\right)\rho_{k-1}\left(\mathbb{1} \otimes B_y^{k-1}\right),
\end{aligned} \tag{24}$$

where $\xi_j = \sqrt{1-\eta_j^2}$ and

$$\mathcal{K}^k_{\pm|y} = \frac{1}{2}\left(\sqrt{\frac{1+\eta_k}{2}} + \sqrt{\frac{1-\eta_k}{2}}\right)\mathbb{1} \pm \frac{1}{2}\left(\sqrt{\frac{1+\eta_k}{2}} - \sqrt{\frac{1-\eta_k}{2}}\right)B^k_y. \quad (25)$$

The quantum value of the Bell functional $\mathcal{I}$ between Alice and Bob^k, $\mathscr{I}^k = \text{Tr}[\mathcal{I}\rho_k]$, is evaluated as (see Appendix B)

$$\mathscr{I}^k = \begin{cases} \eta_1 \sum_{y=1}^3 \omega_y \text{Tr}[\mathscr{A}_y \otimes B_y \rho_1] = \eta_1 \mathscr{I}_{\text{opt}} & \text{if } k=1 \\ \eta_k \sum_{y=1}^3 \omega_y \tilde{\omega}^k_y \text{Tr}\big(\mathscr{A}_y \otimes \mathscr{B}^k_y \rho_{k-1}\big) & \text{if } k \geqslant 2, \end{cases} \quad (26)$$

where $\mathscr{A}_y$ and ω_y are given by Eq. (10), $\mathscr{B}^k_y = \tilde{B}_y{}^k/\tilde{\omega}^k_y$ with $\tilde{\omega}^k_y = \|\tilde{B}^k_y\|_{\rho_{k-1}}$, and

$$\tilde{B}^k_y = \frac{1+\xi_{k-1}}{2} B^k_y + \frac{1-\xi_{k-1}}{6}\sum_{y'=1}^{3} B^{k-1}_{y'} B^k_y B^{k-1}_{y'} \,\forall\, y. \quad (27)$$

Since $\mathscr{I}_{\text{opt}} = 6$, it follows from Eq. (26) that the suboptimal quantum Bell value between Alice and Bob^1 is $\mathscr{I}^1 = 6\eta_1$.

Lemma 1. The suboptimal quantum Bell value between Alice and Bob^1 is $\mathscr{I}^1 = 6\eta_1$ with Bob^1's observable satisfying the condition $B^1_1 + B^1_2 + B^1_3 = 0$, thereby implying $\langle\{B^1_y, B^1_{y'}\}_{y\neq y'}\rangle_{\rho_1} = -1$.

We prove the following theorems.

Theorem 1. If Alice and Bob^1 obtain the suboptimal Bell value of $\mathscr{I}^1 = 6\eta_1$, the suboptimal quantum Bell value between Alice and Bob^2 is $\mathscr{I}^2 = 3\eta_2(1+\sqrt{1-\eta_1^2})$ with both of Bob's observables satisfying the condition $B^k_1 + B^k_2 + B^k_3 = 0$, thereby implying $\langle\{B^k_y, B^k_{y'}\}_{y\neq y'}\rangle_{\rho_1} = -1$ with $k \in \{1,2\}$.

Proof. From Eq. (26) $\mathscr{I}^2$ is

$$\mathscr{I}^2 = \eta_2 \sum_{y=1}^{3} \omega_y \tilde{\omega}^2_y \text{Tr}\big(\mathscr{A}_y \otimes \mathscr{B}^2_y \rho_1\big), \quad (28)$$

where $\mathscr{B}^2_y = \tilde{B}^2_y/\tilde{\omega}^2_y$, $\tilde{\omega}^2_y = \|\tilde{B}^2_y\|_{\rho_1}$, and

$$\tilde{B}^2_y = \frac{1+\xi_1}{2} B^2_y + \frac{1-\xi_1}{6}\sum_{y'=1}^{3} B^1_{y'} B^2_y B^1_{y'} \,\forall\, y. \quad (29)$$

To optimize $\mathscr{I}^2$, we again employ the SOS approach and define a positive operator as

$$\gamma = \frac{1}{2}\sum_{y=1}^{3} \omega_y \tilde{\omega}^2_y L^\dagger_y L_y. \quad (30)$$

The operators L_i are given by

$$L_y = \mathscr{A}_y \otimes \mathbb{1} - \mathbb{1} \otimes \frac{\tilde{B}^2_y}{\tilde{\omega}^2_y}, \quad \tilde{\omega}^2_y = \big\|\tilde{B}^2_y\big\|_{\rho_1} \,\forall\, y \in \{1,2,3\}. \quad (31)$$

Now, similar to the method presented in Sec. III, from Eqs. (30) and (31) we obtain

$$\mathscr{I}^2 = \eta_2 \left(\max \sum_{y=1}^{3} \omega_y \tilde{\omega}^2_y\right) \quad [\because \text{Tr}[\gamma\rho_1] = 0]. \quad (32)$$

Next, invoking the inequality $\sum_y \sqrt{r_y s_y} \leqslant \sqrt{\sum_y r_y}\sqrt{\sum_y s_y}$, we get

$$\mathscr{I}^2 \leqslant \eta_2 \max \sqrt{(\omega_1)^2 + (\omega_2)^2 + (\omega_3)^2} \times \max \sqrt{\left(\tilde{\omega}^2_1\right)^2 + \left(\tilde{\omega}^2_2\right)^2 + \left(\tilde{\omega}^2_3\right)^2}. \quad (33)$$

Note that equality holds when $\omega_y = \omega_{y'}$ and $\tilde{\omega}_y = \tilde{\omega}_{y'}$. From Eq. (13) we already obtained $\max\sqrt{\omega_1^2+\omega_2^2+\omega_3^2} = 2\sqrt{3}$ when $\langle\{A_y, A_{y'}\}_{y\neq y'}\rangle_{\rho_1} = -1$ and $A_1 + A_2 + A_3 = 0$. The optimality condition $\text{Tr}[\gamma\rho_1] = 0$ implies that $\text{Tr}[L_y\rho_1] = 0$. This means that $\mathscr{A}_y \otimes \mathbb{1} = \mathbb{1} \otimes \frac{\tilde{B}^2_y}{\tilde{\omega}^2_y}$. Therefore, $A_1 + A_2 + A_3 = 0$ implies $\tilde{B}^2_1 + \tilde{B}^2_2 + \tilde{B}^2_3 = 0$. By using this relation, we obtain (see Appendix C)

$$\left\langle\left\{B^2_y, B^2_{y'}\right\}_{y\neq y'}\right\rangle_{\rho_1} = -1 \,\forall\, y, y \in \{1,2,3\} \quad (34)$$

and

$$\sum_{y,y'=1}^{3} B^1_{y'} B^2_y B^1_{y'} = 0. \quad (35)$$

Now, using the relation $\tilde{\omega}^2_y = \tilde{\omega}^2_{y'}$ and Eq. (35), we get (see Appendix D)

$$\sum_{y'=1}^{3} B^1_{y'} B^2_y B^1_{y'} = 0 \,\forall\, y \in \{1,2,3\}. \quad (36)$$

Using Eq. (36) in Eq. (29), we arrive at

$$\tilde{B}^2_y = \frac{1+\xi_1}{2} B^2_y. \quad (37)$$

It is evident from Eq. (37) that

$$\tilde{\omega}^2_y = \big\|\tilde{B}^2_y\big\|_{\rho_1} = \frac{1+\xi_1}{2} = \frac{1+\sqrt{1-\eta_1^2}}{2}. \quad (38)$$

Using Eq. (38), the suboptimal quantum Bell value between Alice and Bob^2 is [as derived from Eq. (33)]

$$\mathscr{I}^2 = 3\eta_2\big(1+\sqrt{1-\eta_1^2}\big). \quad (39)$$

■

Theorem 2. If Alice and Bob^1, and Alice and Bob^2 obtain the suboptimal Bell violations, the suboptimal quantum Bell value between Alice and Bob^3 is $\mathscr{I}^3 = \frac{3\eta_3}{2}(1+\sqrt{1-\eta_1^2})(1+\sqrt{1-\eta_2^2})$, with Bob^k's observables satisfying the condition $B^k_1 + B^k_2 + B^k_3 = 0$, thereby implying $\langle\{B^k_y, B^k_{y'}\}_{y\neq y'}\rangle_{\rho_1} = -1$ with $k \in \{1,2,3\}$.

Proof. By using Eq. (24) we can write ρ_2 in terms of ρ_1 and from Eq. (26) we obtain the value of $\mathscr{I}^3$ in terms of ρ_1 as

$$\mathscr{I}^3 = \eta_3 \sum_{y=1}^{3} \omega_y \tilde{\omega}^3_y \text{Tr}\big(\mathscr{A}_y \otimes \mathscr{B}^3_y \rho_1\big), \quad (40)$$

where $\mathscr{B}_y^3 = \frac{\tilde{B}_y^3}{\tilde{\omega}_y^3}$, $\tilde{\omega}_y^3 = \|\tilde{B}_y^3\|_{\rho_1}$, and

$$\tilde{B}_y^3 = \frac{(1+\xi_1)(1+\xi_2)}{4}B_y^3 + \frac{(1-\xi_1)(1+\xi_2)}{12}\sum_{y'=1}^{3} B_{y'}^1 B_y^3 B_{y'}^1 + \frac{(1+\xi_1)(1-\xi_2)}{12}\sum_{y'=1}^{3} B_{y'}^2 B_y^3 B_{y'}^2 + \frac{(1-\xi_1)(1-\xi_2)}{36} \times \sum_{y',y''=1}^{3} B_{y''}^1 B_{y'}^2 B_y^3 B_{y'}^2 B_{y''}^1. \quad (41)$$

From Lemma 1 and Theorem 1 we can see that Bob[1]'s measurement settings and Bob[2]'s measurement settings satisfy the same condition, i.e., $(B_1^k + B_2^k + B_3^k)_{k\in\{1,2\}} = 0$. Then, without loss of generality, we can take $B_y^2 = B_y^1 \; \forall\, y \in \{1,2,3\}$. With this condition $\tilde{B}_y^3$ is simplified as

$$\tilde{B}_y^3 = \frac{(1+\xi_1)(1+\xi_2)}{4}B_y^3 + \frac{(1-\xi_1\xi_2)}{6}\sum_{y'=1}^{3} B_{y'}^1 B_y^3 B_{y'}^1 + \frac{(1-\xi_1)(1-\xi_2)}{36}\sum_{y',y''=1}^{3} B_{y''}^1 B_{y'}^1 B_y^3 B_{y'}^1 B_{y''}^1. \quad (42)$$

To optimize $\mathscr{I}^3$, we follow an approach similar to the proof of Theorem 1. We define a positive operator

$$\gamma = \frac{1}{2}\sum_{y=1}^{3} \omega_y \tilde{\omega}_y{}^3 L_y^\dagger L_y. \quad (43)$$

The operators L_y are defined as

$$L_y = \mathscr{A}_y \otimes \mathbb{1} - \mathbb{1} \otimes \frac{\tilde{B}_y^3}{\tilde{\omega}_y^3}, \quad \tilde{\omega}_y^3 = \left\|\tilde{B}_y^3\right\|_{\rho_1} \forall\, y \in \{1,2,3\}. \quad (44)$$

Then, similar to the argument presented in Theorem 1, we obtain

$$\mathscr{I}^3 \leqslant \eta_3 \max\sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2} \times \max\sqrt{\left(\tilde{\omega}_1^3\right)^2 + \left(\tilde{\omega}_2^3\right)^2 + \left(\tilde{\omega}_3^3\right)^2}, \quad (45)$$

where the equality holds when $\omega_y = \omega_y$ and $\tilde{\omega}_y^3 = \tilde{\omega}_y^3$, leading to the condition $\tilde{B}_1^3 + \tilde{B}_2^3 + \tilde{B}_3^3 = 0$. Invoking this condition, we obtain the relations (see Appendix E)

$$\left\langle \{B_y^3, B_{y'}^3\}_{y\neq y'} \right\rangle_{\rho_1} = -1 \;\forall\, y, y' \in \{1,2,3\}, \quad (46)$$

$$\sum_{y,y'=1}^{3} B_{y'}^1 B_y^3 B_{y'}^1 = \sum_{y,y',y''=1}^{3} B_{y''}^1 B_{y'}^1 B_y^3 B_{y'}^1 B_{y''}^1 = 0. \quad (47)$$

By using the relation $\tilde{\omega}_y^3 = \tilde{\omega}_{y'}^3$ and Eq. (47), we get (see Appendix F)

$$\sum_{y'=1}^{3} B_{y'}^1 B_y^2 B_{y'}^1 = \sum_{y',y''=1}^{3} B_{y''}^1 B_{y'}^1 B_y^3 B_{y'}^1 B_{y''}^1 = 0. \quad (48)$$

Now, by inserting Eq. (48) in Eq. (42), we obtain

$$\tilde{B}_y^3 = \frac{(1+\xi_1)(1+\xi_2)}{4}B_y^3, \quad (49)$$

which in turn gives

$$\tilde{\omega}_y^3 = \left\|\tilde{B}_y^3\right\|_{\rho_1} = \frac{(1+\xi_1)(1+\xi_2)}{4} \;\forall\, y \in \{1,2,3\}. \quad (50)$$

Therefore, from Eqs. (45) and (50), the suboptimal quantum Bell value between Alice and Bob[3] is given by

$$\mathscr{I}^3 = \frac{3\eta_3}{2}\left(1 + \sqrt{1-\eta_1^2}\right)\left(1 + \sqrt{1-\eta_2^2}\right). \quad (51)$$

■

Theorem 3. If Alice and Bob[1], Alice and Bob[2], and Alice and Bob[3] obtain the suboptimal Bell violations, then no further sequential Bob gets the Bell violation.

Proof. From Lemma 1 and Theorems 1 and 2 we prove that Alice and Bob[1], Alice and Bob[2], and Alice and Bob[3] will obtain suboptimal violation if all of Bob's observables satisfy the conditions $B_1^k + B_2^k + B_3^k = 0$ and $\{B_i^k, B_j^k\}_{i\neq j} = -1$ for all $k \in \{1,2,3\}$. Now, without loss of generality, we can always take $B_i^k = B_j^k \;\forall\, k \in \{1,2,3\}$. By using these facts, from Eq. (26) we obtain

$$\mathscr{I}^4 = \frac{3\eta_4}{4}\prod_{j=1}^{3}\left(1 + \sqrt{1-\eta_j^2}\right). \quad (52)$$

Notably, in the context of the Alice-Bob[1] violation, the bound of η_1 satisfies $\frac{2}{3} < \eta_1 \leqslant 1$. Additionally, it is evident that $\frac{2}{3} < \eta_1 < \eta_2 < \eta_3$. Thus, the maximum Bell value achievable by Alice and Bob[4] is given by

$$\mathscr{I}^4 = \frac{3}{4}\left(1 + \frac{\sqrt{5}}{3}\right)^3 \approx 3.9876 < 4. \quad (53)$$

■

To summarize, we have evaluated quantum suboptimal Bell values for Alice and Bob[1] ($\mathscr{I}^1$), Alice and Bob[2] ($\mathscr{I}^2$), and Alice and Bob[3] ($\mathscr{I}^3$). Subsequent sections will elaborate on the way these concurrently suboptimal values play a pivotal role in certifying the unsharp parameters under the condition $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\} > 4$.

V. SELF-TESTING OF UNSHARP QUANTUM INSTRUMENTS

Following Lemma 1 and Theorems 1 and 2, it is evident that Alice and Bob[1], Alice and Bob[2], and Alice and Bob[3] will attain simultaneous violations of the preparation noncontextual bound of the Bell inequality given by Eq. (1) if $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\} > 4$. Now, from Lemma 1 it is deduced that

$$\mathscr{I}^1 > 4 \Rightarrow \frac{2}{3} < \eta_1 \leqslant 1. \quad (54)$$

Likewise, from Theorem 1 we obtain

$$\mathscr{I}^2 > 4 \Rightarrow \frac{4}{3\left(1 + \sqrt{1-\eta_1^2}\right)} < \eta_2 \leqslant 1. \quad (55)$$

It is worth noting that since $0 < \eta_2 \leqslant 1$, Eq. (55) establishes a lower bound for η_2, which consequently fixes the upper bound of η_1. Thus, we have $\frac{2}{3} < \eta_1 \leqslant \frac{2\sqrt{2}}{3}$.

Next Theorem 2 reveals that the suboptimal quantum Bell violation for Alice and Bob[3], i.e., $\mathscr{I}^3 > 4$, imposes constraints on both the upper bound of η_2 and the lower bound of η_3, evaluated as

$$\eta_2 < \frac{4\sqrt{3\sqrt{1-\eta_1^2}-1}}{3\left(1+\sqrt{1-\eta_1^2}\right)}, \tag{56}$$

$$\frac{8}{3\left(1+\sqrt{1-\eta_1^2}\right)\left(1+\sqrt{1-\eta_2^2}\right)} < \eta_3 \leqslant 1. \tag{57}$$

Together with Eqs. (55) and (56), we derive

$$\frac{4}{3\left(1+\sqrt{1-\eta_1^2}\right)} < \eta_2 < \frac{4\sqrt{3\sqrt{1-\eta_1^2}-1}}{3\left(1+\sqrt{1-\eta_1^2}\right)}. \tag{58}$$

Notably, the upper and lower bounds of η_2 consequently restrict the upper bound of η_1, specifically $\eta_1 < \frac{\sqrt{5}}{3}$. Therefore, the lower and upper bounds for η_1 are given by

$$\frac{2}{3} < \eta_1 < \frac{\sqrt{5}}{3}. \tag{59}$$

Hence, for $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\} > 4$ we find the bounds of three unsharpness parameters as given by Eqs. (57)–(59).

From Lemma 1 and Theorem 1 we have $\mathscr{I}^1 = 6\eta_1$ and $\mathscr{I}^2 = 3\eta_2(1+\sqrt{1-\eta_1^2})$. It is evident that an increase in the unsharpness parameter η_1 for Bob[1] leads to a decrease in the suboptimal Bell value between Alice and Bob[2]. This implies that the more Bob[1] extracts information, the less the value of $\mathscr{I}^2$ is obtained. Thus, there exists a trade-off between the suboptimal quantum Bell values for Alice and Bob[1] and for Alice and Bob[2].

Additionally, by applying Theorem 2 and rewriting $\mathscr{I}^3$ in terms of $\mathscr{I}^1$ and $\mathscr{I}^2$, we get

$$\mathscr{I}^3 = \frac{3}{2}\left[1+\sqrt{1-\left(\frac{\mathscr{I}^1}{6}\right)^2}\right] \times \left(1+\sqrt{1-\frac{(\mathscr{I}^2)^2}{9\left[1+\sqrt{1-\left(\frac{\mathscr{I}^1}{6}\right)^2}\right]^2}}\right). \tag{60}$$

The optimal trade-off between the suboptimal quantum bounds of the Bell inequality for Alice and Bob[1], Alice and Bob[2], and Alice and Bob[3] is given by Eq. (60) and illustrated in Fig. 2. It is important to highlight here that $\mathscr{I}^3 > 4$ implies $4 < \mathscr{I}^1 < 2\sqrt{5}$ and $4 < \mathscr{I}^2 < 4\sqrt{\frac{1}{2}\sqrt{36-(\mathscr{I}^1)^2}-1}$. The lower bound of $\mathscr{I}^1$ determines the upper bound of $\mathscr{I}^2$, i.e., $4 < \mathscr{I}^2 < 4\sqrt{\sqrt{5}-1}$.

Now, given that $\frac{\mathscr{I}^1}{42} \ll 1$ and $\frac{\mathscr{I}^2}{42} \ll 1$, we can expand the right-hand side of Eq. (60) using the Taylor series expansion. Furthermore, by neglecting higher-order terms of $\frac{\mathscr{I}^1}{42}$ and $\frac{\mathscr{I}^2}{42}$,

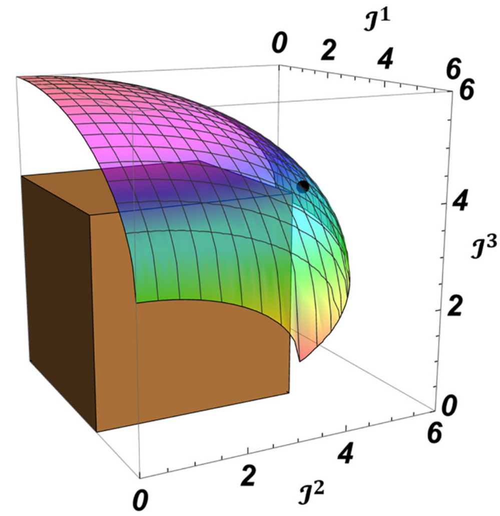

FIG. 2. Graph illustrating the trade-off among the suboptimal quantum bounds for the Bell values between Alice and Bob[1], Alice and Bob[2], and Alice and Bob[3]. The brown-colored cuboid depicts the preparation noncontextual region of the concerned Bell inequality. The colored curved surface indicates the region where the optimal quantum values of the Bell function exceed the preparation noncontextual bound, which is 4. The black point on the three-dimensional graph holds significance as it serves as a crucial point certifying the unsharpness parameters η_1 and η_2 when the quantum values of all three sequential Bobs are considered to be equal. Each point on the curved surface represents a distinct set of sequential Bell values that self-tests a particular set of unsharpness parameters $\{\eta_1, \eta_2\}$.

specifically, taking $O((\frac{\mathscr{I}^1}{42})^m) = O((\frac{\mathscr{I}^2}{42})^m) = 0$ with $m \geqslant 3$ and $O((\frac{\mathscr{I}^1\mathscr{I}^2}{36})^n) = 0$ with $n \geqslant 2$, we derive

$$-(\mathscr{I}^3 - 6) \approx \frac{3}{2}\left[\left(\frac{\mathscr{I}^1}{6}\right)^2 + \left(\frac{\mathscr{I}^2}{6}\right)^2\right]. \tag{61}$$

This equation represents a paraboloid about the negative $\mathscr{I}^3$ axis, with the origin shifted to (6,0,0). We are particularly interested in the region where $\mathscr{I}^k \in [4, 6]$ with $k = \{1, 2, 3\}$ and consider only the half section of the paraboloid, i.e., semiparaboloid.[1]

It is crucial to emphasize that for sharp measurements of Bob_3, meaning $\eta_3 = 1$, each point on the surface of the semiparaboloid in Fig. 2 uniquely certifies the pair (η_1, η_2). For instance, the black point on the surface of the semiparaboloid uniquely certifies ($\eta_1 = \frac{20}{29} \approx 0.69$, $\eta_2 = \frac{4}{5} \approx 0.8$) for $\mathscr{I}^1 = \mathscr{I}^2 = \mathscr{I}^3 = \frac{120}{29} \approx 4.14$.

Self-testing statement in the sequential scenario

From Lemma 1 and Theorems 1 and 2, the optimal tuple $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\}$ uniquely certifies the state shared between

[1]A semiparaboloid is a three-dimensional geometric shape that is formed by taking a paraboloid and cutting it along a plane. It is essentially half of a paraboloid. The term "semi" indicates that only half of the paraboloid is considered, resulting in a curved surface resembling a half bowl or half umbrella.

Alice and Bob^1, along with the observables of both Alice and Bob and the unsharpness parameters of Bob. The self-testing statements are as follows.

(i) The initial shared state between Alice and Bob^1 is a bipartite maximally entangled state in any arbitrary dimension.

(ii) Alice performs projective measurements on her subsystem in any arbitrary local dimension. For the optimal values of the tuple, Alice's observables must satisfy the condition $A_1 + A_2 + A_3 = 0$, revealing a particular anticommutation relation between her observables, given by $\{A_i, A_j\}_{i\neq j} = -1$.

(iii) Bob^k performs unsharp measurements on his subsystem in any arbitrary local dimension, which satisfies the conditions $B_1^k + B_2^k + B_3^k = 0$ and $\{B_i^k, B_j^k\}_{i\neq j} = -1$ for all $k \in \{1, 2, 3\}$.

(iv) The optimal tuple $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\}$ uniquely certifies the pair of unsharpness parameters $\{\eta_1, \eta_2\}$. In other words, the specific values of $\mathscr{I}^1$, $\mathscr{I}^2$, and $\mathscr{I}^3$ allow for a precise determination of the unsharpness parameters η_1 and η_2 associated with the experiment.

VI. ROBUST CERTIFICATION OF THE UNSHARPNESS PARAMETER

Since the experimental demonstration of achieving the tuple $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\}$ is always subject to unavoidable noises and imperfections, here we investigate to what extent the self-testing statements, presented in Sec. V, remain valid and reliable in the presence of such noises. Specifically, when the optimal tuple $\{\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3\}$ cannot be realized, it becomes impossible to uniquely certify the pair $\{\eta_1, \eta_2\}$. Instead, in such instances, it is only possible to certify the ranges of the pair $\{\eta_1, \eta_2\}$.

It is important to note that according to Lemma 1, Alice and Bob^1 obtain a Bell violation when η_1 lies in the range $(\frac{2}{3}, 1]$. Consequently, if $\mathscr{I}^1 > 4$, this implies that $(\eta_1)_{\min} = \frac{2}{3}$. However, the range of η_1 that can be certified will become more restricted when nonlocality is extended further between Alice and Bob^2.

Now, for sequential Bell violation between Alice and Bob^1 and between Alice and Bob^2, i.e., when $\mathscr{I}^1$ and $\mathscr{I}^2$ both exceed 4, we employ Theorem 1 to determine an upper bound of η_1. In this case, with $\eta_2 = 1$, we find that $(\eta_1)_{\max} = \frac{2\sqrt{2}}{3}$. Therefore, the simultaneous Bell violation between Alice and Bob^1 and between Alice and Bob^2 certifies a range of η_1, specifically $\frac{2}{3} < \eta_1 < \frac{2\sqrt{2}}{3}$.

Furthermore, if all three Bobs demonstrate Bell violations with Alice independently, it further narrows down the range of η_1. As a result, the allowed interval for η_1 becomes even more restricted compared to the previous case. In order to evaluate this range, we utilize Eq. (59), which yields the interval $\eta_1 \in (\frac{2}{3}, \frac{\sqrt{5}}{3})$. In addition to this, the presence of Bell violation between Alice and Bob^3 implies a range for η_2, which is given by $\eta_2 \in (3 - \sqrt{5}, \frac{4}{5})$.

Therefore, when Alice and Bob^1, Alice and Bob^2, and Alice and Bob^3 all demonstrate a preparation contextuality bound of the concerned Bell inequality, a particular range for both η_1 and η_2 is certified. In conclusion, if $\mathscr{I}^1, \mathscr{I}^2, \mathscr{I}^3 > 4$, then it is established that η_1 lies in the interval $(\frac{2}{3}, \frac{\sqrt{5}}{3})$ and η_2 lies in the interval $(3 - \sqrt{5}, \frac{4}{5})$.

Finally, by considering the expression (51), we find that $\mathscr{I}^3 > 4$ fixes the lower bound of η_3, which is given by

$$(\eta_3)_{\min} = \frac{2\mathscr{I}^3}{3\left[1 + \sqrt{1 - (\eta_1)^2_{\min}}\right]\left[1 + \sqrt{1 - (\eta_2)^2_{\min}}\right]} = \frac{1}{2}\left(3 + \sqrt{5} - \sqrt{6\sqrt{5} - 2}\right) \approx 0.93. \tag{62}$$

It is essential to underscore that the power of the sequential scenario compared to the usual Bell scenario not only facilitates the certification of the unsharpness parameters but also enables the certification of the incompatibility of sequential measurements.

VII. QUANTIFYING AND CERTIFYING SEQUENTIAL MEASUREMENT INCOMPATIBILITY

The measurement incompatibility in quantum theory gives rise to a wide range of intriguing phenomena such as uncertainty relations [61,67], preparation contextuality [68,69], and state discrimination [70]. Incompatibility is also crucial for comprehending quantum correlations such as quantum steering [63] and nonlocality [32,71,72]. Since incompatible measurements are necessary for demonstrating quantum correlations, sequential violations of the preparation noncontextual bounds of $\mathscr{I}^1$, $\mathscr{I}^2$, and $\mathscr{I}^3$ device-independently certifies that three POVMs for each Bob are incompatible [73]. It should be noted here that using the CHSH inequality, two incompatible POVMs have been certified in the sequential scenario in terms of the degree of incompatibility introduced in [74]. However, such certification assumed the dimension of the state and observables. Here, by suitably quantifying the degree of incompatibility [60,74,75], we first certify the sequential degree of incompatibility for two POVMs in the CHSH scenario. For this purpose, we invoke the recently obtained [4] DI bounds of the CHSH value between Alice and Bob^1 and between Alice and Bob^2. Then we proceed to the certification of the degree of incompatibility of three POVMs.

A. DI sequential certification of the degree of incompatibility of two POVMs

Following [60,74], where qubit observables were assumed, we define the degree of incompatibility between two dichotomic observables in arbitrary dimensions

$$\mathcal{D}(B_1, B_2) = \|B_1 + B_2\| + \|B_1 - B_2\| - 2. \tag{63}$$

All compatible observables obey $\mathcal{D}(B_1, B_2) \leqslant 0$, whereas B_0 and B_1 are incompatible, if $0 < \mathcal{D}(B_1, B_2) \leqslant (2\sqrt{2} - 2)$.

Now considering the CHSH functional [3]

$$\mathscr{C} = A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2) \tag{64}$$

and employing the SOS method introduced in [35], the optimal CHSH value $\mathcal{C} = \mathrm{Tr}[\mathscr{C}\rho]$ also can be expressed as [4]

$$\mathcal{C} \leqslant \|B_1 + B_2\| + \|B_1 - B_2\| = \mathcal{D}(B_1, B_2) + 2. \tag{65}$$

Therefore, B_1 and B_2 will be incompatible if and only if $\mathcal{D}(B_1, B_2) \geqslant \mathcal{C} - 2 > 0$.

In the sequential scenario, the degree of incompatibility of Bob[1]'s observables is given by

$$\mathcal{D}(B_1^1, B_2^1) \geqslant \frac{\mathcal{C}^1}{\eta_1} - 2 \quad (66)$$

Then the measurements of B_1^1 and B_2^1 will be incompatible if and only if $\mathcal{C}^1 > 2$, which in turn fixes the lower bound of η_1, i.e., $\frac{1}{\sqrt{2}} < \eta_1 \leqslant 1$.

The CHSH value between Alice and Bob[2] is evaluated as (see Sec. 3 of [4])

$$\begin{aligned}\mathcal{C}^2 &\leqslant \frac{1}{2}\big(1+\sqrt{1-\eta_1^2}\big)\big[\|B_1^2+B_2^2\| + \|B_1^2-B_2^2\|\big]\\ &= \frac{1}{2}\big(1+\sqrt{1-\eta_1^2}\big)\big[\mathcal{D}(B_1^2, B_2^2)+2\big]. \end{aligned} \quad (67)$$

Thus, the degree of incompatibility of Bob[2]'s observables is given by

$$\mathcal{D}(B_1^2, B_2^2) \geqslant \frac{2\mathcal{C}^2}{1+\sqrt{1-\eta_1^2}} - 2 \quad (68)$$

and B_1^2 and B_2^2 will be incompatible if and only if $\mathcal{C}^2 > 2$. This in turn fixes the upper bound of η_1, i.e., $0 \leqslant \eta_1 < \sqrt{2(\sqrt{2}-1)}$.

Now, to obtain simultaneous CHSH violations between Alice and Bob[1] and between Alice and Bob[2], the degree of incompatibility must be greater than zero, i.e., $\mathcal{D}(B_1^1, B_2^1) > 0$ and $\mathcal{D}(B_1^2, B_2^2) > 0$. These conditions then fix both the upper and lower bounds of Bob[1]'s unsharp parameter η_1, given by

$$\frac{1}{\sqrt{2}} < \eta_1 < \sqrt{2(\sqrt{2}-1)}. \quad (69)$$

From Eqs. (66) and (68) we obtain the trade-off between the degree of incompatibility of Bob[1]'s and Bob[2]'s observables. Note that with increasing values of η_1, while the incompatibility of Bob[1]'s observables decreases, the incompatibility of Bob[2]'s observable increases up to a certain upper bound of $(\eta_1)_{\max} = \sqrt{2(\sqrt{2}-1)}$.

B. DI sequential certification of the degree of incompatibility of three POVMs

The degree of incompatibility between any three dichotomic observables is defined as [60]

$$\begin{aligned}&\mathcal{D}(B_1, B_2, B_3)\\ &\quad = \|B_1+B_2+B_3\| + \|B_1-B_2+B_3\|\\ &\qquad + \|B_1+B_2-B_3\| + \|-B_1+B_2+B_3\| - 4, \end{aligned} \quad (70)$$

where B_1, B_2, and B_3 are incompatible if and only if $0 < \mathcal{D}(B_1, B_2, B_3) \leqslant 4(\sqrt{3}-1)$. The maximum incompatibility bound is saturated if $\{B_i, B_j\}_{i\neq j} = 0$.

However, if we choose B_1, B_2, and B_3 in such a way that they satisfy $B_1 + B_2 + B_3 = 0$ (trine-spin observables), then the degree of incompatibility can be defined as

$$\begin{aligned}\mathcal{D}_T(B_1, B_2, B_3) &= \|B_1-B_2+B_3\| + \|B_1+B_2-B_3\|\\ &\quad + \|-B_1+B_2+B_3\| - 4. \end{aligned} \quad (71)$$

Note that for the case of trine observables, the maximum value of the right-hand side of Eq. (71) is 2 (see Sec. III). Thus, B_1, B_2, and B_3 are incompatible if and only if $0 < \mathcal{D}_T(B_1, B_2, B_3) \leqslant 2$. The maximum incompatibility bound is saturated if $\{B_i, B_j\}_{i\neq j} = -1$.

In order to witness sequential quantum violations, all Bobs must perform a smeared version of a projective measurement, known as unsharp measurement, characterized by the unbiased POVM. Unbiased POVMs are defined by $\mathcal{B}_y \equiv \{\frac{\mathbb{1}\pm\eta B_y}{2}\}$. Consequently, the degree of incompatibility is determined by the unsharpness parameter η. For three anticommuting qubit observables B_y, the $\mathcal{B}'_y$ are jointly measurable or compatible if and only if $\eta \leqslant \frac{1}{\sqrt{3}}$ [60]. In addition, it has been demonstrated that the triplewise joint measurability condition for the smeared version of trine qubit observables is given by $\eta \leqslant \frac{2}{3}$.

Here we first certify the sequential measurement incompatibility between a specific class of three observables, known as trine observables, that satisfy $\sum B_y = 0\,\forall\, y$. Subsequently, using the sequential scenario considered in [4], we generalize our treatment of the certification of the degree of incompatibility for any set of three unbiased POVMs.

DI sequential certification of the degree of incompatibility of trine observables

In the sequential scenario, it is evident from Sec. III that the degree of incompatibility of Bob[1]'s observables is given by

$$\mathcal{D}_T(B_1^1, B_2^1, B_3^1) \geqslant \frac{\mathscr{I}^1}{\eta_1} - 4. \quad (72)$$

Thus, B_1^1, B_2^1, and B_3^1 are incompatible if and only if $\mathscr{I}^1 > 4$, which in turn fixes the lower bound of η_1, i.e., $\frac{2}{3} < \eta_1 \leqslant 1$.

Reexpressing Eq. (1), we arrive at the Bell value between Alice and Bob[2],

$$\mathscr{I}^2 = \eta_2 \sum_{y=1}^{3} \mathrm{Tr}\big(A_y \otimes \mathfrak{B}_y^2 \rho_2\big), \quad (73)$$

where $\mathfrak{B}_1^2 = B_1^2 + B_2^2 - B_3^2$, $\mathfrak{B}_2^1 = B_1^2 - B_2^2 + B_3^2$, and $\mathfrak{B}_3^1 = -B_1^2 + B_2^2 + B_3^2$. By employing the SOS method outlined in Sec. III we obtain

$$\mathscr{I}^2 \leqslant \eta_2 \sum_{y=1}^{3} \big\|\mathfrak{B}_y^2\big\|_{\rho_2}. \quad (74)$$

By evaluating ρ_2 from Eq. (24), we derive

$$\begin{aligned}\mathscr{I}^2 &\leqslant \frac{\eta_2}{2}\big(1+\sqrt{1-\eta_1^2}\big)\sum_{y=1}^{3}\big\|\mathfrak{B}_y^2\big\|_{\rho_1}\\ &= \frac{\eta_2}{2}\big(1+\sqrt{1-\eta_1^2}\big)\big[\mathcal{D}_T(B_1^2, B_2^2, B_3^2)+4\big]. \end{aligned} \quad (75)$$

Thus, the degree of incompatibility of Bob^2's observables is deduced as

$$\mathcal{D}_T\left(B_1^2, B_2^2, B_3^2\right) \geqslant \frac{2\mathscr{I}^2}{\eta_2\left(1+\sqrt{1-\eta_1^2}\right)} - 4. \tag{76}$$

Hence, it follows from Eq. (76) that Bob^2's observables are incompatible if and only if $\mathscr{I}^2 > 4$. Subsequently, the upper bound of η_1 is restricted as $0 \leqslant \eta_1 < \frac{2\sqrt{2}}{3}$ and the lower bound of η_2 is given by $\frac{4}{3(1+\sqrt{1-\eta_1^2})} < \eta_2 \leqslant 1$, which is in conformity with the bound previously found in Sec. VI. Therefore, the minimum value of η_2 is restricted from the lower bound of η_1, which is $\frac{2}{3} < \eta_2 \leqslant 1$.

Note that both Bobs' observables will be incompatible for the ranges $\frac{2}{3} < \eta_1 \leqslant \frac{2\sqrt{2}}{3}$ and $3-\sqrt{5} < \eta_2 \leqslant 1$. An interesting point to be emphasized here is that although Bob^2's observable are incompatible for $\eta_2 > \frac{2}{3}$, in the sequential nature of the experiment, they become compatible in the range $\frac{2}{3} < \eta_2 < 3-\sqrt{5}$. Hence, in the sequential scenario, there exists a trade-off between the degree of incompatibility between Bob^1's and Bob^2's observables.

Similarly, we analyze the sequential degree of incompatibility of Bob^3's observables. For this, we write the Bell value between Alice and Bob^3 as

$$\begin{aligned}\mathscr{I}^3 &= \eta_3 \sum_{y=1}^{3} \mathrm{Tr}\left(A_y \otimes \mathfrak{B}_y^3 \rho_3\right) \\ &\leqslant \eta_3 \sum_{y=1}^{3} \left\|\mathfrak{B}_y^3\right\|_{\rho_3} \\ &\leqslant \frac{\eta_3}{4}\left(1+\sqrt{1-\eta_1^2}\right)\left(1+\sqrt{1-\eta_2^2}\right)\left\|\mathfrak{B}_y^3\right\|_{\rho_1} \\ &= \frac{\eta_3}{4}\left(1+\sqrt{1-\eta_1^2}\right)\left(1+\sqrt{1-\eta_2^2}\right)\left[\mathcal{D}_T\left(B_1^3, B_2^3, B_3^3\right)+4\right].\end{aligned} \tag{77}$$

Therefore, the degree of incompatibility of Bob^3's observables is given by

$$\mathcal{D}_T\left(B_1^3, B_2^3, B_3^3\right) \geqslant \frac{4\mathscr{I}^3}{\eta_3\left(1+\sqrt{1-\eta_1^2}\right)\left(1+\sqrt{1-\eta_2^2}\right)} - 4. \tag{78}$$

Bob^3's observables are incompatible if and only if $\mathscr{I}^3 > 4$, which fixes the lower bound of η_3 and the upper bounds of η_1 and η_2. It then straightforwardly follows that, in order to ensure all three sequential Bobs' observables are incompatible, i.e., $\{\mathcal{D}_T(B_1^k, B_2^k, B_3^k)\} > 0\, \forall\, k \in \{1, 2, 3\}$, the relations between three unsharpness parameters are reproduced as given by Eqs. (57)–(59).

Notably, three sequential Bobs have the same degree of incompatibility for the following values of unsharpness parameters:

$$\eta_1 = \frac{4\eta_3\left(4+\eta_3^2\right)}{16+12\eta_3^2+\eta_3^4}, \quad \eta_2 = \frac{4\eta_3}{4+\eta_3^2}, \\ \times \frac{1}{2}\left(3+\sqrt{5}-\sqrt{6\sqrt{5}-2}\right) \leqslant \eta_3 \leqslant 1. \tag{79}$$

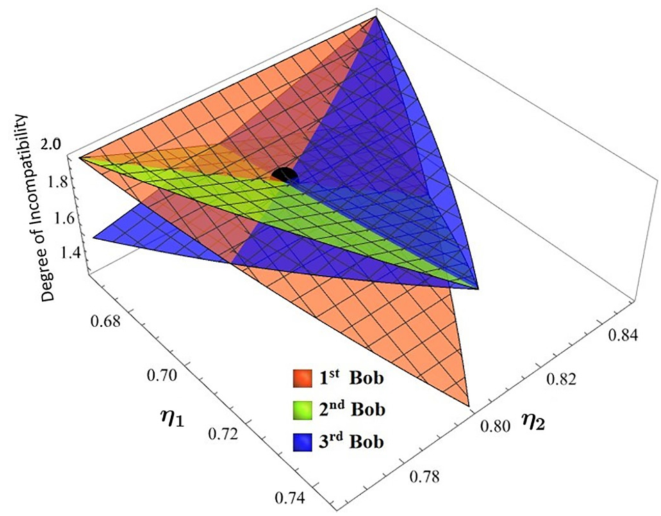

FIG. 3. Graph illustrating the trade-off between the degree of incompatibilities of three Bobs with respect to η_1 and η_2. Here we take $\eta_3 = 1$. The yellow-, blue-, and green-colored planes in the three-dimensional plot illustrate variations of the degree of incompatibility of Bob^1, Bob^2, and Bob^3, respectively. The black point on the three-dimensional graph signifies a particular point where the degree of incompatibility of the three Bobs is the same.

Under such a set of conditions on unsharpness parameters, Bell values between Alice and Bob^1, Alice and Bob^2, and Alice and Bob^3 are identical, given by $\mathscr{I}^k = \frac{24\eta_3(4+\eta_3^2)}{16+12\eta_3^2+\eta_3^4}\, \forall\, k \in \{1, 2, 3\}$. This is anticipated because incompatibility implies the Bell violation. If we take $\eta_3 = 1$, then the values of η_1 and η_2 are $\eta_1 = \frac{20}{29}$ and $\eta_2 = \frac{4}{5}$, leading to $\mathcal{D}_T(B_1^k, B_2^k, B_3^k) = \frac{29\mathscr{I}^k}{20} - 4\, \forall\, k \in \{1, 2, 3\}$. Therefore, it is evident that the same degree of incompatibility implies identical Bell values for Alice and Bob^1, Alice and Bob^2, and Alice and Bob^3. If we choose a specific Bell value, such as $\mathscr{I}^k = \frac{120}{29} \approx 4.14$, the degree of incompatibility becomes 2, signifying that the optimal Bell value corresponds to the maximum degree of incompatibility. The variations between the three Bobs' degrees of incompatibility are illustrated in Fig. 3.

VIII. CONCLUSION

The present study has explored the self-testing of noisy quantum instruments based on the preparation contextual quantum correlations. For this purpose, we employed a specific Bell inequality wherein two spacelike separated parties Alice and Bob perform three measurements each. A notable aspect of such an inequality is its preparation noncontextual bound of 4, which is less than the local bound of 5. Consequently, this offers an advantage in exploiting nonclassicality within a quantum correlation. Using an elegant SOS approach, we derived the optimal quantum violation of this inequality to be 6 devoid of assuming the dimension of the quantum system. Subsequently, based on this optimal bound, the conditions for both party's observables have been established. In particular, the optimal quantum violation self-tests that Alice's and Bob's observables must satisfy the conditions $A_1 + A_2 + A_3 = 0$ and $B_1 + B_2 + B_3 = 0$, respectively. This in turn provides $\langle\{A_i, A_j\}_{i\neq j}\rangle = \langle\{B_i, B_j\}_{i\neq j}\rangle = -1\,\forall\, i, j \in \{1, 2, 3\}$. This particular class of observables is called trine observables if an analogy is drawn with a qubit system. Furthermore, we derived that the shared state must be a maximally entangled state in any dimension.

We provided the self-testing of unsharp quantum instruments based on the suboptimal sequential quantum violations of the Bell inequality. We explicitly demonstrated that at most three sequential Bobs can violate the preparation noncontextuality inequality. As mentioned, the standard Bell test is incapable of self-testing the unsharpness parameter as the effect of the unsharp measurements is reflected in the post-measurement states. Since the suboptimal quantum violations may originate from many different sources, the self-testing of an unsharp quantum instrument inevitably requires the simultaneous DI certification of the state, measurement, and unsharpness parameter. We showed that the suboptimal quantum violations of Alice and Bob^1, Alice and Bob^2, and Alice and Bob^3 form an optimal tuple leading to a trade-off relationship among three sequential violations (illustrated in Fig. 2) and enabling the self-testing of the unsharpness parameters of Bob^1 and Bob^2. This in turn self-tests that the shared state between Alice and Bob^1 must be maximally entangled and all observables of Alice and the three sequential Bobs must satisfy the conditions of trine observables.

Further, we have provided a robust self-testing in a practical experimental scenario involving noise and imperfections. Due to the presence of noise, one may obtain lower values than the predicted suboptimal quantum values of the Bell functional. We demonstrated that in such a case only specific ranges of unsharp parameters can be self-tested, which in turn demonstrates the noise robustness of our protocol.

Finally, by noting that incompatible measurements are necessary for demonstrating preparation contextual quantum correlations [29,30], we investigated the quantification of sequential Bob's degree of incompatibility. Specifically, we introduced an expression for the degree of incompatibility of a trine class of observables. We then evaluated the lower and upper bounds to demonstrate the extent to which the degree of incompatibility affects the bounds of unsharp parameters. The dependence of the degree of incompatibility on unsharp parameters was presented in Fig. 3. This dimension-independent analysis is a significant advancement over prior works and creates possibilities for comprehending the intricate relationships governing quantum correlations.

We remark here that a suboptimal quantum violation of a Bell inequality can occur if the state is not maximally entangled or if both parties' respective measurement operators are not sharp projective measurements. In our present work we have certified the unsharp parameter by introducing the noise to the measurement. On the other hand, recent studies [76,77] have demonstrated to what extent a maximally entangled state can be self-tested from the quantum violation of CHSH inequality in the presence of noise in the shared state. While our approach does not consider noise in the state, as suboptimal sequential violation requires the initial state to be maximally entangled, the works of [76,77] did not consider the noise in the measurement procedure. Thus, extending our dimension-independent framework, it would be worthwhile to investigate the extent to which one can certify a noisy quantum instrument if a noisy channel affects the initial bipartite state.

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APPENDIX A: DERIVATION OF EXPRESSIONS OF $C_i \otimes C_i$ AND PROOFS OF $[C_i \otimes C_i, C_j \otimes C_j]_{i\neq j} = 0$, $\text{Tr}[C_i\rho] = 1$, AND $\text{Tr}[(\mathscr{A}_i \otimes B_i)\rho] = 1$

Here $\text{Tr}[(\mathscr{A}_i \otimes B_i)\rho] = 1$ implies ρ is a pure state. Hence, we rewrite the optimality condition in terms of a pure state $|\psi\rangle$ as

$$\mathscr{A}_i \otimes B_i\,|\psi\rangle = |\psi\rangle\;\forall\, i \in \{1, 2, 3\}. \tag{A1}$$

Now, for $i = 1$, from Eq. (A1) we obtain the following set of relations:

$$\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1\,|\psi\rangle = \mathscr{A}_2 \otimes B_2\,|\psi\rangle \quad \text{[multiplying } \mathscr{A}_2 \otimes B_2 \text{ from the left by Eq. (A1)]}, \tag{A2}$$

$$\mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1\,|\psi\rangle = \mathscr{A}_3 \otimes B_3\,|\psi\rangle \quad \text{[multiplying } \mathscr{A}_3 \otimes B_3 \text{ from the left by Eq. (A1)]}, \tag{A3}$$

$$\mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1\,|\psi\rangle = \mathscr{A}_3 \otimes B_2\,|\psi\rangle \quad \text{[multiplying } \mathscr{A}_3 \otimes B_2 \text{ from the left by Eq. (A1)]}, \tag{A4}$$

$$\mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1\,|\psi\rangle = \mathscr{A}_2 \otimes B_3\,|\psi\rangle \quad \text{[multiplying } \mathscr{A}_2 \otimes B_3 \text{ from the left by Eq. (A1)]}. \tag{A5}$$

First, we consider $C_1 \otimes C_1 = \mathscr{A}_1 \otimes B_1$, thus implying $\text{Tr}[C_1 \otimes C_1\rho] = 1$. Next, for $i = 2$ and $i = 3$, from Eq. (A1) we obtain another set of relations

$$\mathscr{A}_2 \otimes B_3\,|\psi\rangle = \mathbb{1} \otimes B_3B_2\,|\psi\rangle \quad \text{[multiplying } \mathbb{1} \otimes B_3B_2 \text{ from the left by Eq. (A1)]}, \tag{A6}$$

$$\mathscr{A}_3 \otimes B_2\,|\psi\rangle = \mathbb{1} \otimes B_2B_3\,|\psi\rangle \quad \text{[multiplying } \mathbb{1} \otimes B_2B_3 \text{ from the left by Eq. (A1)]}. \tag{A7}$$

Adding $\mathscr{A}_2 \otimes B_2 |\psi\rangle = |\psi\rangle$ with $\mathscr{A}_3 \otimes B_3 |\psi\rangle = |\psi\rangle$ and subtracting with Eqs. (A6) and (A7), we get

$$(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_3 \otimes B_2)|\psi\rangle = (2\mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes\{B_2, B_3\})|\psi\rangle,$$

$$\frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_3 \otimes B_2)|\psi\rangle = |\psi\rangle \quad \text{for } \langle\{B_2, B_3\}\rangle_\rho = -1, \tag{A8}$$

$$\mathrm{Tr}\left[\frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_3 \otimes B_2)\rho\right] = 1. \tag{A9}$$

Next, taking $C_2 \otimes C_2 = \frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_3 \otimes B_2)$, Eq. (A9) simplifies to $\mathrm{Tr}[C_2 \otimes C_2\rho] = 1$. Finally, adding Eqs. (A2) and (A3) as well as subtracting Eqs. (A4) and (A5), we derive

$$(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1)|\psi\rangle = (\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_3 \otimes B_2)|\psi\rangle,$$

$$(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1)|\psi\rangle = 3|\psi\rangle \quad \text{[from (A8)]},$$

$$\mathrm{Tr}\left[\frac{1}{3}(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1)\right] = 1. \tag{A10}$$

We choose $C_3 \otimes C_3 = \frac{1}{3}(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1)$; consequently, $\mathrm{Tr}[C_3 \otimes C_3\rho] = 1$. It is straightforward to obtain that $C_3 \otimes C_3 = (C_2 \otimes C_2)(C_1 \otimes C_1)$. In the following we show that, for $[C_i \otimes C_i, C_j \otimes C_j]_{i\neq j} = 0\,\forall\, i, j \in \{1, 2, 3\}$,

$$\begin{aligned}
[C_1 \otimes C_1, C_3 \otimes C_3] &= \frac{1}{3}[\mathscr{A}_1 \otimes B_1, (\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1)]\\
&= \frac{1}{3}[(\mathscr{A}_1 \otimes B_1)(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1)\\
&\quad -(\mathscr{A}_2\mathscr{A}_1 \otimes B_2B_1 - \mathscr{A}_2\mathscr{A}_1 \otimes B_3B_1 - \mathscr{A}_3\mathscr{A}_1 \otimes B_2B_1 + \mathscr{A}_3\mathscr{A}_1 \otimes B_3B_1)(\mathscr{A}_1 \otimes B_1)]\\
&= \frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_3 \otimes B_2 - \mathscr{A}_2 \otimes B_3 - \mathscr{A}_2 \otimes B_2 - \mathscr{A}_3 \otimes B_3 + \mathscr{A}_3 \otimes B_2 + \mathscr{A}_2 \otimes B_3) = 0.
\end{aligned} \tag{A11}$$

Here, in order to get the third line from the second line, we invoke the relations $\mathscr{A}_1 + \mathscr{A}_2 + \mathscr{A}_3 = B_1 + B_2 + B_3 = 0$ and $\langle\{\mathscr{A}_i, \mathscr{A}_j\}_{i\neq j}\rangle = \langle\{B_i, B_j\}_{i\neq j}\rangle = -1$:

$$\begin{aligned}
[C_1 \otimes C_1, C_2 \otimes C_2] &= \left[\mathscr{A}_1 \otimes B_1, \frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_3 \otimes B_2 - \mathscr{A}_2 \otimes B_3)\right]\\
&= \frac{1}{3}[(\mathscr{A}_1\mathscr{A}_2 \otimes B_1B_2 + \mathscr{A}_1\mathscr{A}_3 \otimes B_1B_3 - \mathscr{A}_1\mathscr{A}_3 \otimes B_1B_2 - \mathscr{A}_1\mathscr{A}_2 \otimes B_1B_3) - (\mathscr{A}_1\mathscr{A}_2 \otimes B_1B_2\\
&\quad +\mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes B_1B_2 + \mathscr{A}_1\mathscr{A}_2 \otimes \mathbb{1} + \mathscr{A}_1\mathscr{A}_3 \otimes B_1B_3 + \mathbb{1}\otimes\mathbb{1} + \mathscr{A}_1\mathscr{A}_3 \otimes \mathbb{1} + \mathbb{1}\otimes B_1B_3 - \mathscr{A}_1\mathscr{A}_3 \otimes B_1B_2\\
&\quad -\mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes B_1B_2 - \mathscr{A}_1\mathscr{A}_3 \otimes \mathbb{1} - \mathscr{A}_1\mathscr{A}_2 \otimes B_1B_3 - \mathbb{1}\otimes\mathbb{1} - \mathbb{1}\otimes B_1B_3 - \mathscr{A}_1\mathscr{A}_2 \otimes \mathbb{1})] = 0.
\end{aligned} \tag{A12}$$

Therefore, from Eqs. (A11) and (A12) and given the condition $C_3 \otimes C_3 = (C_2 \otimes C_2)(C_1 \otimes C_1)$, it follows that $[C_2 \otimes C_2, C_3 \otimes C_3] = 0$. Furthermore, $[C_i \otimes C_i, C_j \otimes C_j]_{i\neq j} = 0$ implies $\mathrm{Tr}[C_i \otimes C_i\rho] = \mathrm{Tr}[C_j \otimes C_j\rho] = 1$.

Next, with such a construction of $C_i \otimes C_i$ as a function of $\mathscr{A}_y \otimes B_y$, we demonstrate that the optimal conditions of Alice's and Bob's observables can be recovered. Let us first recall the expression of the bipartite state ρ from Eq. (19),

$$\rho = \frac{1}{d^2}\left(\mathbb{1}_d \otimes \mathbb{1}_d + C_1 \otimes C_1 + C_2 \otimes C_2 + C_3 \otimes C_3 + \sum_{i=4}^{d^2-1} C_i \otimes C_i\right). \tag{A13}$$

Now, in order to proof the relation $\mathrm{Tr}[\mathscr{A}_y \otimes B_y\rho] = 1$, we need some additional conditions on $\mathscr{A}_y$ and B_y. At the optimal condition, these relations are $\{\mathscr{A}_i, \mathscr{A}_j\}_{i\neq j} = \{B_i, B_j\}_{i\neq j} = -\mathbb{1}_d$, which directly implies $\mathrm{Tr}[B_iB_j]_{\imath\neq j} = \mathrm{Tr}[\mathscr{A}_i\mathscr{A}_j]_{i\neq j} = -\frac{d}{2}$ and $\mathrm{Tr}[\sum_{i=4}^{d^2-1} \mathscr{A}_jC_i \otimes B_jC_i] = 0\,\forall\, j = 1, 2, 3$:

$$\mathrm{Tr}[(\mathscr{A}_1 \otimes B_1)\rho] = \frac{1}{d^2}\mathrm{Tr}\left[\mathscr{A}_1 \otimes B_1 + \mathbb{1}_d \otimes \mathbb{1}_d + \frac{1}{3}(\mathscr{A}_2 \otimes B_2 + \mathscr{A}_3 \otimes B_3 - \mathscr{A}_3 \otimes B_2 - \mathscr{A}_2 \otimes B_3 + \mathscr{A}_1\mathscr{A}_2 \otimes B_1B_2)\right]$$

$$+\frac{1}{d^2}\mathrm{Tr}\left(\frac{1}{3}(\mathscr{A}_1\mathscr{A}_3\otimes B_1B_3-\mathscr{A}_1\mathscr{A}_3\otimes B_1B_2-\mathscr{A}_1\mathscr{A}_2\otimes B_1B_3)+\sum_{i=4}^{d^2-1}\mathscr{A}_1C_i\otimes B_1C_i\right)$$

$$=\frac{1}{d^2}\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]+\frac{1}{3d^2}\left(\frac{d^2}{4}-\frac{d^2}{4}-\frac{d^2}{4}+\frac{d^2}{4}\right)=\frac{1}{d^2}\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]=1, \tag{A14}$$

$$\mathrm{Tr}[(\mathscr{A}_2\otimes B_2)\rho]=\frac{1}{d^2}\mathrm{Tr}\bigg[\mathscr{A}_2\otimes B_2+\mathscr{A}_2\mathscr{A}_1\otimes B_2B_1+\frac{1}{3}(\mathbb{1}_d\otimes\mathbb{1}_d+\mathscr{A}_2\mathscr{A}_3\otimes B_2B_3-\mathscr{A}_2\mathscr{A}_3\otimes\mathbb{1}_d-\mathbb{1}_d\otimes B_2B_3+\mathscr{A}_1\otimes B_1)\bigg]$$

$$-\frac{1}{d^2}\mathrm{Tr}\left(\frac{1}{3}(\mathscr{A}_1\otimes B_2B_3B_1-\mathscr{A}_2\mathscr{A}_3\mathscr{A}_1\otimes B_1+\mathscr{A}_2\mathscr{A}_3\mathscr{A}_1\otimes B_2B_3B_1)+\sum_{i=4}^{d^2-1}\mathscr{A}_2C_i\otimes B_2C_i\right)$$

$$=\frac{1}{d^2}\left(\frac{d^2}{4}+\frac{3\,d^2}{4}\right)\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]=\frac{1}{d^2}\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]=1, \tag{A15}$$

$$\mathrm{Tr}[(\mathscr{A}_3\otimes B_3)\rho]=\frac{1}{d^2}\mathrm{Tr}\bigg[\mathscr{A}_3\otimes B_3+\mathscr{A}_3\mathscr{A}_1\otimes B_3B_1+\frac{1}{3}(\mathbb{1}_d\otimes\mathbb{1}_d+\mathscr{A}_3\mathscr{A}_2\otimes B_3B_2-\mathscr{A}_3\mathscr{A}_2\otimes\mathbb{1}_d-\mathbb{1}_d\otimes B_3B_2+\mathscr{A}_1\otimes B_1)\bigg]$$

$$-\frac{1}{d^2}\mathrm{Tr}\left(\frac{1}{3}(\mathscr{A}_1\otimes B_3B_2B_1-\mathscr{A}_3\mathscr{A}_2\mathscr{A}_1\otimes B_1+\mathscr{A}_3\mathscr{A}_2\mathscr{A}_1\otimes B_3B_2B_1)+\sum_{i=4}^{d^2-1}\mathscr{A}_3C_i\otimes B_3C_i\right)$$

$$=\frac{1}{d^2}\left(\frac{d^2}{4}+\frac{3\,d^2}{4}\right)\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]=\frac{1}{d^2}\mathrm{Tr}[\mathbb{1}_d\otimes\mathbb{1}_d]=1. \tag{A16}$$

APPENDIX B: EVALUATION OF THE BELL VALUE BETWEEN ALICE AND BOB^k

The reduced state after the $(k-1)$th Bob's measurement is evaluated as

$$\rho_k=\frac{1+\xi_{k-1}}{2}\rho_{k-1}+\frac{1-\xi_{k-1}}{6}\sum_{y=1}^{3}\big(\mathbb{1}\otimes B_y^{k-1}\big)\rho_1\big(\mathbb{1}\otimes B_y^{k-1}\big). \tag{B1}$$

Now the Bell value between Alice and Bob^k is given by

$$\mathscr{I}^k=\mathrm{Tr}[\mathcal{I}\rho_k]=\eta_k\mathrm{Tr}\big\{\big[(A_1+A_2-A_3)\otimes B_1^k+(A_1-A_2+A_3)\otimes B_2^k+(-A_1+A_2+A_3)\otimes B_3^k\big]\rho_k\big\}$$

$$=\eta_k\sum_{y=1}^{3}\omega_y\mathrm{Tr}\big(\mathscr{A}_y\otimes B_y^k\rho_k\big)\quad\text{[from Eq. (10)]}$$

$$=\eta_k\frac{1+\xi_{k-1}}{2}\sum_{y=1}^{3}\omega_y\mathrm{Tr}\big(\mathscr{A}_y\otimes B_y^k\rho_{k-1}\big)+\eta_k\frac{1-\xi_{k-1}}{6}\sum_{y=1}^{3}\omega_y\mathrm{Tr}\left[\mathscr{A}_y\otimes\left(\sum_{y'=1}^{3}B_{y'}^{k-1}B_y^kB_{y'}^{k-1}\right)\rho_{k-1}\right]$$

$$=\eta_k\sum_{y=1}^{3}\omega_y\mathrm{Tr}\big(\mathscr{A}_y\otimes\tilde{B}_y^k\rho_{k-1}\big)\quad\text{with }\tilde{B}_y^k=\frac{1+\xi_{k-1}}{2}B_y^k+\frac{1-\xi_{k-1}}{6}\sum_{y'=1}^{3}B_{y'}^{k-1}B_y^kB_{y'}^{k-1}\ \forall\, y\in\{1,2,3\}. \tag{B2}$$

APPENDIX C: PROOF OF EQS. (34) AND (35)

The condition $\tilde{B}_1^2+\tilde{B}_2^2+\tilde{B}_3^2=0$ implies

$$\frac{1+\xi_1}{4}\big(B_1^2+B_2^2+B_3^3\big)+\frac{1-\xi_1}{6}\sum_{y,y'=1}^{3}B_{y'}^1B_y^2B_{y'}^1=0\quad\text{[from Eq. (B2)]}. \tag{C1}$$

Since B_y^2 and $B_i^1B_y^2B_i^1$ are independent of the quantity ξ_1, the left-hand side of Eq. (C1) can be made zero by ensuring that both of the coefficient of ξ_1 and ξ_1^0 are simultaneously zero. This leads to the conditions

$$B_1^2+B_2^2+B_3^3=\frac{2}{3}\sum_{y,y'=1}^{3}B_{y'}^1B_y^2B_{y'}^1,\quad B_1^2+B_2^2+B_3^3=-\frac{2}{3}\sum_{y,y'=1}^{3}B_{y'}^1B_y^2B_{y'}^1. \tag{C2}$$

Therefore, Eq. (C2) implies

$$B_1^2 + B_2^2 + B_3^3 = 0, \quad \sum_{y,y'=1}^{3} B_{y'}^1 B_y^2 B_{y'}^1 = 0. \tag{C3}$$

It is then evident that $B_1^2 + B_2^2 + B_3^2 = 0$ implies $\langle \{B_i^2, B_j^2\}_{i\neq j}\rangle_{\rho_1} = -1$.

APPENDIX D: PROOF OF EQ. (36)

The maximization condition $\tilde{\omega}_1^2 = \tilde{\omega}_2^2$ results in $\|\tilde{B}_1^2\|_{\rho_1} = \|\tilde{B}_2^2\|_{\rho_1}$, implying $\mathrm{Tr}[\tilde{B}^2{}_1^\dagger \tilde{B}^2{}_1\rho_1] = \mathrm{Tr}[\tilde{B}^2{}_2^\dagger \tilde{B}^2{}_2\rho_1]$. Recalling the quantities $\tilde{B}_y^2$ from Eq. (B2), we infer

$$\sum_{y=1}^{2}(-1)^{1+y}\left(6\big(1-\xi_1^2\big)\left\langle\left\{B_y^2, \sum_{y'=1}^{3} B_{y'}^1 B_y^2 B_{y'}^1\right\}\right\rangle_{\rho_1} + (1-\xi_1)^2\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_y^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_y^2 B_{y'}^1\right\}\right\rangle_{\rho_1}\right) = 0. \tag{D1}$$

Now comparing the coefficients of ξ_1 from both sides of Eq. (D1), we get

$$\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = \left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1\right\}\right\rangle_{\rho_1}. \tag{D2}$$

At the maximization condition of $\mathscr{I}^2$ as stated in Theorem 1, we have $\tilde{\omega}_i^2 = \tilde{\omega}_j^2$ and $\tilde{B}_1^2 + \tilde{B}_2^2 + \tilde{B}_3^2 = 0$. This condition satisfies $\langle\{\frac{\tilde{B}_i^2}{\tilde{\omega}_i^2}, \frac{\tilde{B}_j^2}{\tilde{\omega}_j^2}\}_{i\neq j}\rangle_{\rho_1} = -1$, given that $\tilde{B}_i^2$ and $\tilde{B}_j^2$ are not normalized. Hence, we express

$$\big\langle\{\tilde{B}_i^2, \tilde{B}_j^2\}_{i\neq j}\big\rangle_{\rho_1} = -\|\tilde{B}_i^2\|^2 = -\|\tilde{B}_j^2\|^2. \tag{D3}$$

Taking $\langle\{\tilde{B}_1^2, \tilde{B}_2^2\}\rangle_{\rho_1} = -\|\tilde{B}_1^2\|^2$, we obtain

$$\begin{aligned}&\frac{1-\xi_1^2}{12}\left\langle\left\{B_1^2, \sum_{y'=1}^{3} B_{y'}^1\big(B_1^2 + B_2^2\big)B_{y'}^1\right\} + \left\{B_2^2, \sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1\right\}\right\rangle_{\rho_1} + \frac{(1-\xi_1)^2}{36}\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1\right\}\right.\\ &\left.+\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = 0.\end{aligned} \tag{D4}$$

In Eq. (D4), B_1^2, B_2^2, and B_3^2 are independent of $(\xi_1)^0$, $(\xi_1)^1$, and $(\xi_1)^2$. Therefore, the coefficients of $(\xi_1)^0$, $(\xi_1)^1$, and $(\xi_1)^2$ must all be zero. The coefficient $\xi_1 = 0$ implies

$$\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1\right\} + \left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = 0. \tag{D5}$$

The expression can be rewritten as

$$\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 (B_1^2 + B_2^2) B_{y'}^1\right\}\right\rangle_{\rho_1} = \left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_3^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = 0. \tag{D6}$$

Likewise, by using $\langle\{\tilde{B}_1^2, \tilde{B}_2^2\}\rangle_{\rho_1} = -\|\tilde{B}_2^2\|^2$, we find

$$\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_3^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = 0. \tag{D7}$$

From other pairs of $\tilde{B}_1^2$ and $\tilde{B}_3^2$ and of $\tilde{B}_2^2$ and $\tilde{B}_3^2$ we obtain

$$\left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_3^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = \left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_3^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = \left\langle\left\{\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1, \sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1\right\}\right\rangle_{\rho_1} = 0. \tag{D8}$$

With the help Eq. (D8) and subsequently squaring Eq. (C2), we arrive at

$$\left(\sum_{y'=1}^{3} B_{y'}^1 B_1^2 B_{y'}^1\right)^2 + \left(\sum_{y'=1}^{3} B_{y'}^1 B_2^2 B_{y'}^1\right)^2 + \left(\sum_{y'=1}^{3} B_{y'}^1 B_3^2 B_{y'}^1\right)^2 = 0. \tag{D9}$$

From Eq. (D2) it follows that

$$\left(\sum_{y'=1}^{3} B^1_{y'}B^2_1B^1_{y'}\right)^2 = \left(\sum_{y'=1}^{3} B^1_{y'}B^2_2B^1_{y'}\right)^2 = \left(\sum_{y'=1}^{3} B^1_{y'}B^2_3B^1_{y'}\right)^2. \tag{D10}$$

Hence, combining Eqs. (D9) and (D10), we obtain

$$\left(\sum_{y'=1}^{3} B^1_{y'}B^2_1B^1_{y'}\right)^2 = \left(\sum_{y'=1}^{3} B^1_{y'}B^2_2B^1_{y'}\right)^2 = \left(\sum_{y'=1}^{3} B^1_{y'}B^2_3B^1_{y'}\right)^2 = 0. \tag{D11}$$

Finally, from Eqs. (D2) and Eq. (D11) we deduce

$$\sum_{y'=1}^{3} B^1_{y'}B^2_1B^1_{y'} = \sum_{y'=1}^{3} B^1_{y'}B^2_2B^1_{y'} = \sum_{y'=1}^{3} B^1_{y'}B^2_3B^1_{y'} = 0. \tag{D12}$$

APPENDIX E: PROOF OF EQS. (46) AND (47)

The maximization of $\mathscr{I}^3$ needs $\sum_{y=1}^{3} \tilde{B}^3_y = 0$ to be satisfied. This in turn gives the relationship [refer to Eq. (42)]

$$\sum_{y=1}^{3}\Bigg[\left(\frac{B^3_y}{4} + \sum_{y'=1}^{3}\frac{B^1_{y'}B^3_yB^1_{y'}}{6} + \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right) + (\xi_1+\xi_2)\left(\frac{B^3_y}{4} - \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right)$$
$$+\xi_1\xi_2\left(\frac{B^3_y}{4} + \sum_{y'=1}^{3}\frac{B^1_{y'}B^3_yB^1_{y'}}{6} - \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right)\Bigg] = 0. \tag{E1}$$

As B^3_y, $B^1_{y'}B^2_yB^1_{y'}$, and $B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}$ are independent of the quantities ξ_1, ξ_2, and $\xi_1\xi_2$, the coefficients of ξ_1, ξ_2, $\xi_1\xi_2$, and $(\xi_1\xi_2)^0$ must be zero. This leads to the relations

$$\sum_{y=1}^{3}\left(\frac{B^3_y}{4} + \sum_{y'=1}^{3}\frac{B^1_{y'}B^3_yB^1_{y'}}{6} + \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right) = 0, \tag{E2}$$

$$\sum_{y=1}^{3}\left(\frac{B^3_y}{4} - \sum_{y'=1}^{3}\frac{B^1_{y'}B^3_yB^1_{y'}}{6} + \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right) = 0, \tag{E3}$$

$$\sum_{y=1}^{3}\left(\frac{B^3_y}{4} - \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right) = 0. \tag{E4}$$

Subtracting and adding Eqs. (E2) and (E3), we evaluate the conditions

$$\sum_{y,y'=1}^{3} B^1_{y'}B^3_yB^1_{y'} = 0, \tag{E5}$$

$$\sum_{y=1}^{3}\left(\frac{B^3_y}{4} + \sum_{y',y''=1}^{3}\frac{B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''}}{36}\right) = 0. \tag{E6}$$

Adding and subtracting Eqs. (E4) and (E6) implies

$$B^3_1 + B^3_2 + B^3_3 = 0, \tag{E7}$$

$$\sum_{y,y',y''=1}^{3} B^1_{y''}B^1_{y'}B^3_yB^1_{y'}B^1_{y''} = 0. \tag{E8}$$

Therefore, it is evident that the condition $B^3_1 + B^3_2 + B^3_3 = 0$ obtained in Eq. (E7) leads to $\langle\{B^3_i, B^3_j\}_{i\neq j}\rangle_{\rho_1} = -1$.

APPENDIX F: PROOF OF EQ. (48)

The maximization condition $\tilde{\omega}_1^3 = \tilde{\omega}_2^3$ implies $\|\tilde{B}_1^3\|_{\rho_1} = \|\tilde{B}_2^2\|_{\rho_1}$, which further leads to $\mathrm{Tr}[\tilde{B}^{2\dagger}_1\tilde{B}^2{}_1\rho_1] = \mathrm{Tr}[\tilde{B}^{2\dagger}_2\tilde{B}^2{}_2\rho_1]$. Recalling the quantities $\tilde{B}_y^3$ from Eq. (42), we arrive at the expressions

$$\sum_{y=1}^{2}(-1)^{1+y}\Bigg(\frac{(1+\xi_1)(1+\xi_2)(1-\xi_1\xi_2)}{24}\left\langle\left\{B_y^3,\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1\right\}\right\rangle_{\rho_1}+\frac{(1-\xi_1^2)(1-\xi_2^2)}{144}\left\langle\left\{B_y^3,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}$$
$$+\frac{(1-\xi_1\xi_2)^2}{36}\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1,\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1\right\}\right\rangle_{\rho_1}+\frac{(1-\xi_1)(1-\xi_2)(1-\xi_1\xi_2)}{216}\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}$$
$$+\frac{(1-\xi_1)^2(1-\xi_2)^2}{36^2}\left\langle\left\{\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}\Bigg)=0. \tag{F1}$$

Comparing the coefficient of ξ_1 and $\xi_1(\xi_2)^2$ from both sides of Eq. (F1), we get

$$\sum_{y=1}^{2}(-1)^{1+y}\left(27\left\langle\left\{B_y^3,\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1\right\}\right\rangle_{\rho_1}-3\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}\right)$$
$$=\sum_{y=1}^{2}(-1)^{1+y}\left(\left\langle\left\{\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}\right), \tag{F2}$$

$$\sum_{y=1}^{2}(-1)^{1+y}\left(-27\left\langle\left\{B_y^3,\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1\right\}\right\rangle_{\rho_1}+3\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_y^3B_{y'}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}\right)$$
$$=\sum_{y=1}^{2}(-1)^{1+y}\left(\left\langle\left\{\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_y^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}\right). \tag{F3}$$

Adding Eqs. (F2) and (F3), we evaluate

$$\left\langle\left\{\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_1^3B_{y'}^1B_{y''}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_1^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}=\left\langle\left\{\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_2^3B_{y'}^1B_{y''}^1,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_2^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}. \tag{F4}$$

Now comparing the coefficient of $\xi_1\xi_2$ from both sides of Eq. (F1) and using Eq. (F4), it is straightforward to obtain the relation

$$\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_1^3B_{y'}^1,\sum_{y'=1}^{3}B_{y'}^1B_1^3B_{y'}^1\right\}\right\rangle_{\rho_1}=\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_2^3B_{y'}^1,\sum_{y'=1}^{3}B_{y'}^1B_2^3B_{y'}^1\right\}\right\rangle_{\rho_1}. \tag{F5}$$

At the maximization condition of $\mathscr{I}^3$ as stated in Theorem 2, we have $\tilde{\omega}_i^3 = \tilde{\omega}_j^3$ and $\tilde{B}_1^3+\tilde{B}_2^3+\tilde{B}_3^3=0$, which satisfies $\langle\{\frac{\tilde{B}_i^3}{\tilde{\omega}_i^3},\frac{\tilde{B}_j^3}{\tilde{\omega}_j^3}\}_{i\neq j}\rangle_{\rho_1}=-1$ as $\tilde{B}_i^3$ and $\tilde{B}_j^3$ are not normalized. Hence, we deduce

$$\langle\{\tilde{B}_i^3,\tilde{B}_j^3\}_{i\neq j}\rangle_{\rho_1}=-\|\tilde{B}_i^3\|^2=-\|\tilde{B}_j^3\|^2. \tag{F6}$$

Taking $\langle\{\tilde{B}_1^3,\tilde{B}_2^3\}\rangle_{\rho_1}=-\|\tilde{B}_1^3\|^2$, we derive the equation

$$\frac{(1+\xi_1)(1+\xi_2)(1-\xi_1\xi_2)}{24}\left\langle\left\{B_1^3,\sum_{y'=1}^{3}B_{y'}^1\big(B_1^3+B_2^3\big)B_{y'}^1\right\}+\left\{B_2^3,\sum_{y'=1}^{3}B_{y'}^1B_1^3B_{y'}^1\right\}\right\rangle_{\rho_1}+\frac{\big(1-\xi_1^2\big)\big(1-\xi_2^2\big)}{144}$$
$$\times\left\langle\left\{B_1^3,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1\big(B_1^3+B_2^3\big)B_{y'}^1B_{y''}^1\right\}+\left\{B_2^3,\sum_{y',y''=1}^{3}B_{y''}^1B_{y'}^1B_1^3B_{y'}^1B_{y''}^1\right\}\right\rangle_{\rho_1}$$
$$\times+\frac{(1-\xi_1\xi_2)^2}{36}\left\langle\left\{\sum_{y'=1}^{3}B_{y'}^1B_1^3B_{y'}^1,\sum_{y'=1}^{3}B_{y'}^1\big(B_1^3+B_2^3\big)B_{y'}^1\right\}\right\rangle_{\rho_1}$$

$$+\frac{(1-\xi_1)(1-\xi_2)(1-\xi_1\xi_2)}{216}\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}\left(B^3_1+B^3_2\right)B^1_{y'}B^1_{y''}\right\}+\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_2B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}$$
$$+\frac{(1-\xi_1)^2(1-\xi_2)^2}{36^2}\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}\left(B^3_1+B^3_2\right)B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=0. \quad \text{(F7)}$$

As $\sum_{y=1}^{3}B^3_y=0$, we arrive at

$$\frac{(1+\xi_1)(1+\xi_2)(1-\xi_1\xi_2)}{24}\left\langle\left\{B^3_2,\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'}\right\}-\left\{B^3_1,\sum_{y'=1}^{3}B^1_{y'}B^3_3B^1_{y'}\right\}\right\rangle_{\rho_1}+\frac{\left(1-\xi_1^2\right)\left(1-\xi_2^2\right)}{144}\left\langle\left\{B^3_2,\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''}\right\}\right.$$
$$\left.-\left\{B^3_1,\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}-\frac{(1-\xi_1\xi_2)^2}{36}\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\sum_{y'=1}^{3}B^1_{y'}B^3_3B^1_{y'}\right\}\right\rangle_{\rho_1}+\frac{(1-\xi_1)(1-\xi_2)(1-\xi_1\xi_2)}{216}$$
$$\times\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_2B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''}\right\}-\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}-\frac{(1-\xi_1)^2(1-\xi_2)^2}{36^2}$$
$$\times\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=0. \quad \text{(F8)}$$

In Eq. (F7), as B^3_1, B^3_2, and B^3_3 are independent of ξ_2, ξ_1, $\xi_1(\xi_2)^2$, and $\xi_1\xi_2$, the coefficients of ξ_2, ξ_1, $\xi_1(\xi_2)^2$, and $\xi_1\xi_2$ must all be equal to zero. From Eq. (F7) the coefficient of $\xi_1=0$ implies

$$27\left\langle\left\{B^3_1,\sum_{y'=1}^{3}B^1_{y'}B^3_3B^1_{y'}\right\}-\left\{B^3_2,\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'}\right\}\right\rangle_{\rho_1}-3\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right.$$
$$\left.-\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_2B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}. \quad \text{(F9)}$$

From Eq. (F7) the coefficient of $\xi_1(\xi_2)^2=0$ implies

$$-27\left\langle\left\{B^3_1,\sum_{y'=1}^{3}B^1_{y'}B^3_3B^1_{y'}\right\}-\left\{B^3_2,\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'}\right\}\right\rangle_{\rho_1}+3\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right.$$
$$\left.-\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_2B^1_{y'},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}. \quad \text{(F10)}$$

Adding Eqs. (F9) and (F10), we derive

$$\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_1B^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_3B^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=0. \quad \text{(F11)}$$

Now, following the similar procedure for obtaining Eq. (F11) and taking into account the other pairs of B^3_1 and B^3_2, and B^3_2 and B^3_2, we arrive at the condition

$$\left\langle\left\{\sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_mB^1_{y'}B^1_{y''},\ \sum_{y',y''=1}^{3}B^1_{y''}B^1_{y'}B^3_nB^1_{y'}B^1_{y''}\right\}\right\rangle_{\rho_1}=0,\quad m\neq n,\ \{m,n\}\in\{1,2,3\}. \quad \text{(F12)}$$

Comparing the coefficients of $\xi_1\xi_2$ from Eq. (F7) and putting them into Eq. (F11), we obtain

$$\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\sum_{y'=1}^{3}B^1_{y'}\left(B^3_1+B^3_2\right)B^1_{y'}\right\}\right\rangle_{\rho_1}=0\quad\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_1B^1_{y'},\sum_{y'=1}^{3}B^1_{y'}B^3_3B^1_{y'}\right\}\right\rangle_{\rho_1}=0. \quad \text{(F13)}$$

Similarly to Eq. (F13), considering other pairs of B^3_m and B^3_n, we derive

$$\left\langle\left\{\sum_{y'=1}^{3}B^1_{y'}B^3_mB^1_{y'},\sum_{y'=1}^{3}B^1_{y'}B^3_nB^1_{y'}\right\}\right\rangle_{\rho_1}=0,\quad m\neq n,\ \{m,n\}\in\{1,2,3\}. \quad \text{(F14)}$$

Using Eq. (F14) and squaring Eq. (E5), we deduce

$$\left\langle \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{1}^{3} B_{y'}^{1} \right)^{2} + \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{2}^{3} B_{y'}^{1} \right)^{2} + \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{3}^{3} B_{y'}^{1} \right)^{2} \right\rangle_{\rho_1} = 0. \tag{F15}$$

Now, from Eqs. (F5) and (F15) it is evident that

$$\left\langle \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{1}^{3} B_{y'}^{1} \right)^{2} \right\rangle_{\rho_1} = \left\langle \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{2}^{3} B_{y'}^{1} \right)^{2} \right\rangle_{\rho_1} = \left\langle \left(\sum_{y'=1}^{3} B_{y'}^{1} B_{3}^{3} B_{y'}^{1} \right)^{2} \right\rangle_{\rho_1}. \tag{F16}$$

Hence, from Eqs. (F15) and (F16) it is straightforward to obtain that

$$\left\langle \sum_{y'=1}^{3} B_{y'}^{1} B_{y}^{2} B_{y'}^{1} \right\rangle_{\rho_1} = 0 \, \forall \, y \in \{1, 2, 3\}. \tag{F17}$$

With the help of Eq. (F12) and squaring of Eq. (E8), we evaluate

$$\left\langle \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{1}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2} + \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{2}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2} + \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{3}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2} \right\rangle_{\rho_1} = 0. \tag{F18}$$

Next Eqs. (F4) and (F18) lead to the relation

$$\left\langle \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{1}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2} \right\rangle_{\rho_1} = \left\langle \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{2}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2} \right\rangle_{\rho_1} = \left\langle \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{3}^{3} B_{y'}^{1} B_{y''}^{1} \right)^{2})^{2} \right\rangle_{\rho_1}. \tag{F19}$$

Finally, from Eqs. (F18) and (F19) we show that

$$\left\langle \left(\sum_{y',y''=1}^{3} B_{y''}^{1} B_{y'}^{1} B_{y}^{3} B_{y'}^{1} B_{y''}^{1} \right) \right\rangle_{\rho_1} = 0 \, \forall \, y \in \{1, 2, 3\}. \tag{F20}$$

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