Incompatibility of observables as state-independent bound of uncertainty relations

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For a pair of observables, they are called "incompatible" if and only if their commutator does not vanish, which represents one of the key features in quantum mechanics. The question is, how can we characterize the incompatibility among three or more observables? Here, we explore one possible route towards this goal through uncertainty relations, which impose fundamental constraints on the measurement precisions for incompatible observables. Specifically, we propose to measure the incompatibility by the optimal state-independent bounds of additive variance-based uncertainty relations. In this way, the degree of incompatibility becomes an intrinsic property among the operators, i.e., state independent. In particular, we focus on the incompatibility of spin-1/2 systems as an illustration. For an arbitrary, including nonorthogonal, setting of a finite number Pauli-spin operators, the incompatibility is analytically solved; the spins are maximally incompatible if and only if they are orthogonal to each other. On the other hand, our measure of incompatibility represents a versatile tool for applications such as testing the entanglement of bipartite states, and EPR-steering criteria.

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I. INTRODUCTION

As a distinguished aspect of the quantum theory, uncertainty relations (URs) [1-5] represent a fundamental limitation on the measurements of physical systems; it is generally impossible to simultaneously measure two complementary observables of a physical system without an "uncertainty." Furthermore, uncertainty relations manifest many intrinsic discrepancies between classical and quantum mechanics, leading to applications such as entanglement detection [6,7], nonlocality of quantum systems [8], EPR-steering criteria [9-13], etc.

One of the most well-known uncertainty relations, between a pair of bounded operators M_1 and M_2 , was formulated in terms of a commutator, $[M_1, M_2] \equiv M_1 M_2 - M_2 M_1$, by Robertson [4] in 1929,

$$\Delta M_1 \Delta M_2 \geqslant \frac{1}{2} |\langle \psi | [M_1, M_2] | \psi \rangle|, \tag{1}$$

where $\Delta M_i \equiv (\langle M_i^2 \rangle - \langle M_i \rangle^2)^{1/2}$ is the standard deviation for the quantum state $|\psi\rangle$. This uncertainty relation appears in almost every textbook of quantum mechanics, and is regarded

as fundamental, connecting the physical concept of incompat*ibility* of observables (IOs) with quantum *uncertainty*.

However, Robertson's inequality cannot be regarded as complete for describing the connection between incompatibility and uncertainty. What if the state $|\psi\rangle$ is an eigenstate of M_1 or M_2 ? The left-hand side becomes zero, which makes no difference if M_1 and M_2 are incompatible or not. Another problem occurs when $|\psi\rangle$ is an eigenstate of the commutator associated with an eigenvalue zero, making the inequality trivial. These problems point to the idea that incompatibility cannot be quantified properly by uncertainty relations when they depend on quantum states [14].

To avoid such problems, Deutsch [14] proposed that URs should be expressed in a state-independent form,

$$\mathcal{U}(M_1, M_2, |\psi\rangle) \geqslant \mathcal{B}(M_1, M_2), \tag{2}$$

where the functional \mathcal{U} denotes the total uncertainty, and \mathcal{B} labels a *tight* state-independent bound. Here, \mathcal{B} only depends on observables M_1 , M_2 and the functional form \mathcal{U} , and hence it measures the intrinsic incompatibility between the two observables. State-independent URs have been investigated from an information-theoretic perspective [13,15–34]. For example, \mathcal{U} can be taken to be the sum of entropies of different bases of measurements (say, $\{|u_i\rangle\}$) and $\{|v_i\rangle\}$), and the lower bound \mathcal{B} is given by functions of the overlap of the basis vectors, $c(i, j) \equiv |\langle u_i | v_i \rangle|^2$. As a second example,

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consider a pair of Pauli-spin operators $S_{\vec{n}_i}$ and $S_{\vec{n}_j}$ pointing to different directions labeled by unit vectors $\vec{n}_{i,j}$, where $S_{\vec{n}_{i,j}} \equiv \vec{n}_{i,j} \cdot \vec{\sigma}$. The optimal state-independent bound for the additive variance-based UR, $\Delta^2 S_{\vec{n}_i} + \Delta^2 S_{\vec{n}_j}$, is given [35] by

$$\min_{\alpha} \left(\Delta^2 S_{\vec{n}_i} + \Delta^2 S_{\vec{n}_j} \right) = 1 - |\vec{n}_i \cdot \vec{n}_j| \equiv \mathcal{I}(\vec{n}_i, \vec{n}_j). \tag{3}$$

The spin operators are compatible ($\mathcal{I}=0$), whenever $\vec{n}_i \cdot \vec{n}_j = 1$, and are maximally incompatible (\mathcal{I} is maximized), whenever they are orthogonal to each other, i.e., $\vec{n}_i \cdot \vec{n}_j = 0$.

Generalizing the above observation, we propose to measure the incompatibility among three or more observables by the optimal state-independent bound \mathcal{B} . In order to give a proper measure, the functional form \mathcal{U} should be suitably chosen. Clearly, the multiplicative variance-based \mathcal{U} in Eq. (1) fails to give a proper incompatibility measure \mathcal{B} . Nevertheless, proper bounds can be given by the additive variance-based UR, as well as the entropic UR. As an illustration, we focus on the variance-based UR in this paper. In particular, for an arbitrary, including nonorthogonal, setting of a finite number Pauli-spin operators $\{S_{\bar{n}_i}\}$, their incompatibility $\mathcal{I}(\{S_{\bar{n}_i}\})$ is analytically solved in spin-1/2 systems. Generalizations to higher-dimensional systems and for entropic URs can be made in future studies.

As a measure of incompatibility, the value of \mathcal{B} depends on the choice of the functional form \mathcal{U} . Therefore, this notion of incompatibility intimately relates to preparational uncertainty relations. In this way, it differs from the traditional incompatibility measure for a collection of measurements [36]. With our notion of incompatibility measure, different criteria for entanglement and EPR-steering detection can be given. Therefore, this notion of incompatibility measure connects incompatibility, uncertainty relations, and quantum correlations, and can be used as a versatile tool for investigating the foundational questions of quantum mechanics.

Notably, Bush *et al.* have defined the incompatibility between two measurements by the optimal state-independent bound of Heisenberg's error-disturbance relation [35]. However, due to the intrinsic nature of the error-disturbance relations, their result is limited to only two measurements. In contrast, using preparational uncertainty relations, our definition is also applicable to three or more observables.

II. SETTING THE STAGE

We first focus on determining the incompatibility for an arbitrary finite set of 2×2 Hermitian observables, through variance-based preparational uncertainty relations. We shall later present some of the results associated with spin operators. First of all, any Hermitian operator M_j can be parametrized by a number and a not necessarily normalized three-dimensional (3D) vector, denoted by a_j and \vec{n}_j , respectively. Explicitly, $M_j = a_j I + \vec{n}_j \cdot \vec{\sigma}$, where \vec{n}_j is not assumed to be normalized. For any given density matrix ρ , it can be parametrized by $\rho = (I + \vec{r} \cdot \vec{\sigma})/2$. Therefore,

$$\Delta^2 M_i = \text{tr}(M_i^2 \rho) - \text{tr}^2(M_i \rho) = (\vec{n}_i \cdot \vec{n}_i) - (\vec{n}_i \cdot \vec{r})^2, \quad (4)$$

which means that the variance is independent of the value of the constant a_j . In other words, we can instead consider the variances of a group of nonorthogonal spin operators

 $S_{\vec{n}_i} \equiv \vec{n}_j \cdot \vec{\sigma}$, i.e.,

$$\sum_{i} \Delta^{2} M_{j} \Leftrightarrow \sum_{i} \Delta^{2} S_{\vec{n}_{j}}.$$
 (5)

This result is consistent with the notion of characterizing compatibility with a commutator, $[M_i, M_j] = [\vec{n}_i \cdot \vec{\sigma}, \vec{n}_j \cdot \vec{\sigma}]$, which is also independent of the values of a_i and a_j .

The next goal is to determine the incompatibility of the observables of nonorthogonal spins,

$$\mathcal{I}(\vec{n}_1, \vec{n}_2, \dots, \vec{n}_N) \equiv \min_{\rho} \sum_{j=1}^{N} \Delta^2 S_{\vec{n}_j}, \tag{6}$$

where the number of terms N > 1 is any finite integer larger than 1. For a special case of three spins N = 3, and all spin operators are orthogonal among one another, e.g., $\{S_x, S_y, S_z\}$, it is known [6] that

$$\Delta^2 S_x + \Delta^2 S_y + \Delta^2 S_z \geqslant 2,\tag{7}$$

which can be saturated by any pure state of a qubit. We shall see how to recover this result as a special case.

Let us consider again a general density matrix of a qubit, $\rho = (I + \vec{r} \cdot \vec{\sigma})/2$, where $\vec{r} = (x, y, z)$ is a normalized vector, together with $\operatorname{tr}(S_{\vec{n}_i}\rho) = \vec{n}_i \cdot \vec{r}$ and $\operatorname{tr}(S_{\vec{n}_i}^2\rho) = n_i^2$, where \vec{n}_i does not need to be normalized. First, in terms of the vector \vec{r} of ρ , we have

$$\min_{\rho} \sum_{i=1}^{N} \Delta^{2} S_{\vec{n}_{i}} = \tau_{1} - \max_{\vec{r}} \sum_{i=1}^{N} (\vec{n}_{i} \cdot \vec{r})^{2}, \tag{8}$$

where $\tau_1 \equiv \sum_{i=1}^{N} (\vec{n}_j \cdot \vec{n}_j)$ does not depend on \vec{r} . It can be shown that the minimum value of the total uncertainty, over all qubit states with the constraints $||\vec{r}|| = 1$, equals

$$\min_{\rho} \sum_{i=1}^{N} \Delta^2 S_{\vec{n}_i} = \tau_1 - \lambda_{\max}(A), \tag{9}$$

where $\lambda_{max}(A)$ is the maximal eigenvalue of a 3×3 matrix Hermitian operator A defined by

$$A \equiv \sum_{i=1}^{N} |\vec{n}_i\rangle\langle\vec{n}_i|,\tag{10}$$

where we have adopted the Dirac notation to denote vectors with three real elements, e.g., $|\vec{n}_i\rangle \equiv \vec{n}_i = (n_{ix}, n_{iy}, n_{iz})^{\top}$. In this way, we can write $\langle \vec{n}_i | \vec{n}_j \rangle = \langle \vec{n}_j | \vec{n}_i \rangle = \vec{n}_i \cdot \vec{n}_j$.

For example, let us first consider the special case with two nonorthogonal spins, \vec{n}_1 and \vec{n}_2 , i.e., N=2. The eigenvalue equation is given by $|\vec{n}_1\rangle\langle\vec{n}_1|\vec{r}\rangle+|\vec{n}_2\rangle\langle\vec{n}_2|\vec{r}\rangle=\lambda|\vec{r}\rangle$, resulting in the largest eigenvalue as

$$\lambda_{\max}(A) = \frac{1}{2} \left[\tau_1 + \sqrt{\left(n_1^2 - n_2^2\right)^2 + 4(\vec{n}_1 \cdot \vec{n}_2)^2} \right], \tag{11}$$

where $\tau_1 = (\vec{n}_1 \cdot \vec{n}_1) + (\vec{n}_2 \cdot \vec{n}_2)$. In the case of Pauli spins, where $||\vec{n}_1|| = ||\vec{n}_2|| = 1$, we have $\lambda_{\max}(A) = 1 + |\vec{n}_1 \cdot \vec{n}_2|$, which reduces to the result presented earlier in Eq. (3).

For three or more spins, we again need to calculate the maximum eigenvalue of A, given by the determinant equation, $\det (\lambda I - A) = 0$, or explicitly, the largest root of

$$\lambda^3 - \tau_1 \lambda^2 - \lambda (\tau_2 - \tau_1^2)/2 - \det(A) = 0,$$
 (12)

where $\tau_k \equiv \operatorname{tr}(A^k)$ for k=1,2,3. In fact, we can express the determinant, $\det A$, in terms of the τ 's only, i.e., $\det A = (\tau_1^3 + 2\tau_3 - 3\tau_1\tau_2)/6$. Therefore, the characteristic equation can be completely determined by the values of the τ 's. Explicitly, they are given by (i) $\tau_1 = \sum_{i=1}^N (\vec{n}_i \cdot \vec{n}_i)$, (ii) $\tau_2 = \sum_{i,j=1}^N (\vec{n}_i \cdot \vec{n}_j)^2$, and (iii) $\tau_3 = \sum_{i,j,k=1}^N (\vec{n}_i \cdot \vec{n}_j)(\vec{n}_j \cdot \vec{n}_k)(\vec{n}_k \cdot \vec{n}_i)$. Therefore, we should expect that the solution of the above equation (12), and also the lower bound of the uncertainty relations, depends only on the products of $\vec{n}_i \cdot \vec{n}_j$, which is consistent with Eq. (3).

To find the largest root, we simplify the above cubic equation [Eq. (12)] by introducing $z \equiv \lambda - \tau_1/3$, leading to

$$z^3 - 3\alpha^2 z - 2\beta = 0, (13)$$

where $\alpha = \sqrt{(3\tau_2 - \tau_1^2)/18}$, and $\beta \equiv \tau_1^3/27 + \tau_3/6 - \tau_1\tau_2/6$. Since this equation is equivalently the characteristic equation of a Hermitian operator A, whose eigenvalues must be real numbers, we conclude that this simplified cubic equation [Eq. (13)] must also have three real roots. In general, for a cubic equation $z^3 + pz + q$ with three real roots, we have the following trigonometric solution,

$$z_k = 2\sqrt{-\frac{p}{3}}\cos\left[\frac{1}{3}\arccos\left(\frac{3q}{2p}\sqrt{\frac{-3}{p}}\right) - \frac{2\pi k}{3}\right], \quad (14)$$

where k=0,1,2. Since the range of arccos is $[0,\pi]$, we can conclude that z_0 is the largest root among the three. Applying this to our equation, with $p=-3\alpha^2$ and $q=-2\beta$, we have $\lambda_{\max}(A)=\tau_1/3+z_0$, leading to our following main results.

III. MAIN RESULTS

To illustrate that the incompatibilities among multiple observables can be measured by the optimal state-independent bound of uncertainty relations, we focus on the additive variance-based UR for qubits. By minimizing the sum of variance $\sum_{j=1}^{N} \Delta^2 M_{n_j}$, the incompatibility $\mathcal{I}(\{M_j\})$ is analytically calculated for an arbitrary finite set of 2×2 Hermitian observables $M_j = a_j I + \vec{n}_j \cdot \vec{\sigma}$, with a_j being a number, $\vec{\sigma}$ being the Pauli matrices, and \vec{n}_j being an normalized 3D vector, which equals

$$\mathcal{I}(\{M_j\}) \equiv \frac{2\tau_1}{3} - 2\alpha \cos\left[\frac{1}{3}\arccos\left(\frac{\beta}{\alpha^3}\right)\right], \quad (15)$$

where $\alpha = \sqrt{(3\tau_2 - \tau_1^2)/18}$, $\beta \equiv \tau_1^3/27 + \tau_3/6 - \tau_1\tau_2/6$, and τ 's are defined as above. From the formula, the incompatibility among 2×2 Hermitian observables only depends on $\vec{n}_i \cdot \vec{n}_j$, which captures the geometric overlap between observables, and is irrelevant to the background noise a_j in each observable. We defer the full proof of our main result to Appendix A.

Especially, if all the vectors \vec{n}_i are normalized, i.e., $||\vec{n}_i|| = 1$ for all observables M_j , we have $\tau_1 = N$, $\tau_2 = N + 2 \sum_{i < j} (\vec{n}_i \cdot \vec{n}_j)^2$, and $\tau_3 = 3\tau_2 - 2N + 6 \sum_{i < j < k} (\vec{n}_i \cdot \vec{n}_j) (\vec{n}_j \cdot \vec{n}_k) (\vec{n}_k \cdot \vec{n}_i)$, and the incompatibility

is given by

$$\mathcal{I}(\{M_j\}) \equiv \frac{2N}{3} - 2\alpha \cos\left[\frac{1}{3}\cos^{-1}\left(\frac{\beta}{\alpha^3}\right)\right], \quad (16)$$

where

$$\alpha^2 = \frac{1}{3} \left[\sum_{1 \le j < h \le N} (\vec{n}_j \cdot \vec{n}_h)^2 - N(N-3)/6 \right], \tag{17}$$

and

$$\beta = \sum_{h < j < t} (\vec{n}_h \cdot \vec{n}_j)(\vec{n}_t \cdot \vec{n}_h)(\vec{n}_j \cdot \vec{n}_t)$$

$$-\frac{1}{3}(N-3) \sum_{j < h} (\vec{n}_j \cdot \vec{n}_h)^2 + \frac{1}{54}N(N-3)(2N-3).$$
(18)

In particular, for three nonorthogonal spins (N = 3), we have

$$\alpha^2 = [(\vec{n}_1 \cdot \vec{n}_2)^2 + (\vec{n}_2 \cdot \vec{n}_3)^2 + (\vec{n}_1 \cdot \vec{n}_3)^2]/3 \tag{19}$$

as the mean value of the products of $(\vec{n}_i \cdot \vec{n}_i)^2$, and

$$\beta = (\vec{n}_1 \cdot \vec{n}_2)(\vec{n}_2 \cdot \vec{n}_3)(\vec{n}_1 \cdot \vec{n}_3), \tag{20}$$

which implies that the incompatibility, or the minimal uncertainty, for three nonorthogonal spins is given by

$$\min_{\rho} \sum_{i=1}^{3} \Delta^2 S_{n_i} = 2 - 2\alpha \cos \left[\frac{1}{3} \cos^{-1} \left(\frac{\beta}{\alpha^3} \right) \right]. \tag{21}$$

This result can be reduced to the previous result (7), if we choose all spin directions to be orthogonal to one another, i.e., $(\vec{n}_1, \vec{n}_2, \vec{n}_3) = (\hat{x}, \hat{y}, \hat{z})$. Notably, this quantity is geometrical in the sense that it depends only on the mutual angles (inner product) between each pair of observables.

IV. APPLICATIONS

We continue by discussing some instructive applications in entanglement and steering detection. First, the use of uncertainty arguments to study entanglement is well known [6]. However, their arguments are based on an unknown global minimum. With our results, the analytic expression for qubit systems can be derived. In the following, we begin by reviewing the entanglement detection via uncertainty relations in detail.

Consider incompatible observables $S_{\vec{n}_i}$: If there is no simultaneous eigenstate of all $S_{\vec{n}_i}$, there must be a nontrivial lower limit \mathcal{B} for the sum of the uncertainties,

$$\sum_{i} \Delta^{2} S_{\vec{n}_{i}} \geqslant \mathcal{B}, \tag{22}$$

while the bound \mathcal{B} is defined as the absolute minimum of the uncertainty sum for any quantum state. It therefore represents a universally valid limitation of the measurement statistics of quantum systems.

In general, a bipartite quantum system between Alice and Bob can be characterized by the assemblages of incompatible observables, $\{S_{\vec{n}_i}\}_i$ and $\{S_{\vec{n}_j}\}_j$, with the sum uncertainty relations formulated by

$$\sum_{i} \Delta^{2} S_{\vec{n}_{j}} \geqslant \mathcal{B}'. \tag{23}$$

Denote the index j as the result of some permutation π , i.e., $j = \pi(i)$, then the measurement statistics of separable states are limited by the following uncertainty relation,

$$\sum_{i} \Delta^{2} \left(S_{\vec{n}_{i}} \otimes I + I \otimes S_{\vec{n}_{\pi(i)}} \right) \geqslant \mathcal{B} + \mathcal{B}', \tag{24}$$

which holds for all possible permutations.

To derive a experimentally feasible criterion for entanglement, \mathcal{B} and \mathcal{B}' must have a specific expression. Here, we can overcome this challenge easily. To show this, we consider IOs on three incompatible observables. Take measurements $S_{\bar{n}_i}$ and $S_{\bar{m}_i}$ working on bipartite systems, respectively, then for separable states, the measurement values are uncorrelated and the total uncertainties are limited by the sum of the local uncertainties

$$\sum_{i=1}^{3} \Delta^{2} \left(S_{\vec{n}_{i}} \otimes I + I \otimes S_{\vec{m}_{i}} \right)$$

$$\geqslant \mathcal{I}(\vec{n}_{1}, \vec{n}_{2}, \vec{n}_{3}) + \mathcal{I}(\vec{m}_{1}, \vec{m}_{2}, \vec{m}_{3}). \tag{25}$$

Any violation of (25) therefore proves that the measured quantum state cannot be separated, since entanglement describes quantum correlations that are more precise than the ones represented by mixtures of product states. Hence the sum of the incompatibility forms a sufficient condition for the existence of entanglement directly.

Next, we consider the EPR-steering scenario [37]: Alice and Bob have local access to subsystems of a bipartite quantum state ρ . Alice chooses one of her measurements a with outcomes A, and similar for Bob. Then a no-EPR-steering model for Bob is

$$p(A, B|a, b) = \sum_{\lambda} p(\lambda)p(A|a, \lambda)p_{Q}(B|b, \lambda), \qquad (26)$$

with probability distributions $p(A|a, \lambda)$ and $p(\lambda)$ under a "hidden variable" λ [38], and $p_Q(B|b, \lambda)$ represents probability distributions for outcomes B which are compatible with a quantum state.

Following Ref. [10], if Alice tries to infer the outcomes of Bob's measurements through measurements on her subsystem, we denote by $B_{\rm est}(A)$ Alice's estimate of the value of Bob's measurement b as a function of the outcomes of her measurement a. The corresponding average inference variance of B given estimate $B_{\rm est}(A)$ is defined by

$$\Delta_{\inf}^{2}(B) = \langle [B - B_{\text{est}}(A)]^{2} \rangle, \tag{27}$$

and its minimum is

$$\Delta_{\min}^{2}(B) = \langle [B - \langle B \rangle_{A}]^{2} \rangle, \tag{28}$$

where the mean $\langle B \rangle_A$ is over the conditional probability p(B|A). Under the no-EPR-steering model, we can derive a bound for $\Delta_{\inf}^2(B)$ [10],

$$\Delta_{\inf}^{2}(B) \geqslant \Delta_{\min}^{2}(B) \geqslant \sum_{\lambda} p(\lambda) \Delta_{Q}^{2}(B|\lambda),$$
(29)

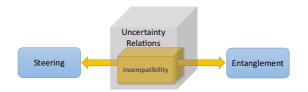


FIG. 1. The core of uncertainty relations is the incompatibility of the observables or measurement, playing the role of a state-independent bound. Such a bound can be employed for detecting quantum entanglement and EPR steering.

where $\Delta_Q^2(B|\lambda)$ represents the probability for *B* predicted by a quantum state ρ_{λ} . Consequently, we can derive the following uncertainty relations for the no-EPR-steering model,

$$\sum_{j=1}^{N} \Delta_{\inf}^{2} \left(S_{\vec{n}_{j}} \right) \geqslant \mathcal{I}(\vec{n}_{1}, \dots, \vec{n}_{N}). \tag{30}$$

Since the above inequality follows directly from assuming a no-EPR-steering model, its violation implies the nonexistence of the local-hidden-state (LHS) model for the outcome statistics. In other words, any violation of the above inequality works as a sufficient condition for EPR steering. Notably, the lower bound is exactly the incompatibility $\mathcal{I}(\vec{n}_1, \ldots, \vec{n}_m)$ for Alice's observables. For qubits, applying our main results, Eq. (15) gives the analytic criteria for EPR steering.

Actually, the formalism of this criterion is based on the conditional probabilities P(B|A) [10]. However, if Alice and Bob take measurements A_j and $S_{\vec{n}_j}$ on their own states, respectively [39], a bipartite state is steerable (from Alice to Bob) if the following uncertainty relations,

$$\sum_{i=1}^{N} \Delta^{2} \left(\alpha_{j} A_{j} \otimes I + I \otimes S_{\vec{n}_{j}} \right) \geqslant \mathcal{I}(\vec{n}_{1}, \dots, \vec{n}_{N}), \tag{31}$$

are violated, and $\{\alpha_j\}$ are arbitrary real numbers. In all of the above we have shown the strength of steerability is determined by the strength of preparation uncertainty in measurements. What really matters in all these applications is the lower bound of the uncertainty relation, i.e., the incompatibility $\mathcal{I}(\vec{n}_1, \ldots, \vec{n}_N)$, and none of these applications would have been possible without the help of the incompatibility. As a consequence, the concepts of uncertainty, entanglement, and EPR steering are naturally linked through the incompatibility $\mathcal{I}(\vec{n}_1, \ldots, \vec{n}_N)$ (see Fig. 1).

V. CONCLUSION

Uncertainty relations can, in principle, be employed to witness quantum correlations, such as entanglement, Bell nonlocality, and EPR steering. However, behind these applications there is a common pattern: the violation of local uncertainty relations as a signature of the quantum correlations. Thus, for each of the applications one has to determine the uncertainty bounds, and this requires a better depiction of the incompatibility of observables. In this paper, we provided a method for determining the optimal uncertainty bounds for any set of 2×2 observables, and their closed form is also obtained, which translates the potential consequences of uncertainty relations

into practice. Moreover, the possibility to use finite arbitrary observables greatly increases the versatility of the detection of quantum correlations.

This work focuses on variance only; it provides us with a particular perspective of the incompatibility under consideration—the perspective that is most relevant to the direct use in an increasing number of experiments that reach the uncertainty-limited regime. Future investigations can be made to extend our results to higher dimensions as well as quantifying the incompatibility by using various forms of uncertainty relations [40], such as entropic uncertainty relations and weighted uncertainty relations (see Appendix B for a more detailed discussion). It is also an interesting open problem to figure out the relationship between our notion of incompatibility measure and many other definitions [36,41]. Another important direction of investigation is the connections between the incompatibility and the non-Markovianity [42]. These are particularly important in the context of open quantum systems [43].

Our work established intriguing connections among a number of fascinating subjects, including quantum foundations, uncertainty principle, quantum correlations, and the geometry of quantum state space, which are of interest to researchers from diverse fields. Uncertainty relations are nothing but mathematical manifestations of the incompatibility of observables, and that is why both entropic uncertainty relations and variance-based uncertainty relations can be used to detect entanglement and characterize steering. Note that compared with previous developments on approximating the optimal bound [44], our method provides an analytical expression of the optimal bound for qubit states.

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APPENDIX A: THE LOWER BOUND OF UNCERTAINTIES

In this Appendix, we first show the direct relation between the eigenvalues of a matrix and its trace through the following lemmas.

Lemma 1. For a 3×3 matrix $A=(a_{jk})_{3\times3}$, its determinant is determined by the following trace formula,

$$Det(A) = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32}$$
$$-a_{12}a_{21}a_{33} - a_{13}a_{22}a_{13} - a_{11}a_{23}a_{23}$$
$$= \frac{1}{6}[Tr^{3}(A) + 2Tr(A^{3}) - 3Tr(A)Tr(A^{2})].$$
(A1)

Lemma 2. For any matrix $M = \sum_{k} |\hat{n}_{k}\rangle \langle \hat{n}_{k}|\hat{n}_{k}$ where \hat{n}_{h} are all real vectors, then we have

$$\tau_{1} := \operatorname{Tr}(M) = \operatorname{Tr}\left(\sum_{k} |\hat{n}_{k}\rangle\langle\hat{n}_{k}|\right) := N, \qquad (A2)$$

$$\tau_{2} := \operatorname{Tr}(M^{2}) = \operatorname{Tr}\left(\sum_{kj} |\hat{n}_{k}\rangle\langle\hat{n}_{k}||\hat{n}_{j}\rangle\langle\hat{n}_{j}|\right)$$

$$= \operatorname{Tr}\left(\sum_{kj} \langle\hat{n}_{j}||\hat{n}_{k}\rangle\langle\hat{n}_{k}||\hat{n}_{j}\rangle\right) = N + 2\sum_{k < j} (\hat{n}_{j} \cdot \hat{n}_{k})^{2}, \qquad (A3)$$

$$\tau_{3} := \operatorname{Tr}(M^{3}) = \operatorname{Tr}\left(\sum_{hjk} |\hat{n}_{h}\rangle\langle\hat{n}_{h}|\hat{n}_{j}\rangle\langle\hat{n}_{j}|\hat{n}_{k}\rangle\langle\hat{n}_{k}|\right)$$

$$= \operatorname{Tr}\left(\sum_{hjk} \langle\hat{n}_{k}|\hat{n}_{h}\rangle\langle\hat{n}_{h}|\hat{n}_{j}\rangle\langle\hat{n}_{j}|\hat{n}_{k}\rangle\right)$$

$$= N + 6\sum_{k < j} (\hat{n}_{j} \cdot \hat{n}_{k})^{2}$$

$$+ 6\sum_{k < j < k} (\hat{n}_{h} \cdot \hat{n}_{j})(\hat{n}_{h} \cdot \hat{n}_{k})(\hat{n}_{j} \cdot \hat{n}_{k}). \qquad (A5)$$

It is also possible to derive the eigenvalues of M which is the root of $Det(M - \lambda I)$, since the value of Det(M) depends on the $Tr(M^k)$, i.e., $6 Det(M) = Tr^3(M) + 2 Tr(M^3) - 3 Tr(M)Tr(M^2)$.

Lemma 3. For $Det(M - \lambda I)$, we have

$$Tr(M - \lambda I) = N - 3\lambda, \tag{A6}$$

$$Tr[(M - \lambda I)^2] = Tr(M^2) - 2N\lambda + 3\lambda^2, \tag{A7}$$

$$Tr[(M - \lambda I)^3] = Tr(M^3) - 3Tr(M^2)\lambda + 3N\lambda^2 - 3\lambda^3.$$
 (A8)

Lemma 4. The largest root of $x^3 + 3\alpha^2 x + 2\beta = 0$ is

$$x = 2|\alpha|\cos\left[\frac{1}{3}\cos^{-1}\left(\frac{\beta}{|\alpha|^3}\right)\right]. \tag{A9}$$

Based on all these lemmas, $\mathcal{I}(\{M_i\})$ can be formulated as

$$\mathcal{I}(\{M_j\}) = N - \lambda = \frac{2N}{3} - t = \frac{2N}{3}$$
$$-2\alpha \cos\left[\frac{1}{3}\cos^{-1}\left(\frac{\beta}{\alpha^3}\right)\right], \quad (A10)$$

with

$$\alpha = \sqrt{\frac{1}{3} \left[\sum_{1 \le j < h \le N} (\vec{n}_j \cdot \vec{n}_h)^2 - N(N-3)/6 \right]}, \quad (A11)$$

and

$$\beta = \sum_{h < j < t} (\vec{n}_h \cdot \vec{n}_j)(\vec{n}_t \cdot \vec{n}_h)(\vec{n}_j \cdot \vec{n}_t)$$

$$-\frac{1}{3}(N-3)\sum_{j < h} (\vec{n}_j \cdot \vec{n}_h)^2 + \frac{1}{54}N(2N-3)(N-3).$$
(A12)

Therefore, the variance-based uncertainty relation with observables M_i reads

$$\sum_{j} \Delta^{2} M_{j} \geqslant \min_{\rho} \sum_{j} \Delta^{2} M_{j} \equiv \mathcal{I}(\{M_{j}\}). \tag{A13}$$

Proof. For any matrix $M = \sum_{k} |\hat{n}_{k}\rangle\langle\hat{n}_{k}|\hat{n}_{k}$, define

$$\tau_k := \operatorname{Tr}(M^k), \tag{A14}$$

then the smallest eigenvalue is given by the following equation,

$$6 \operatorname{Det}(M - \lambda I) = \operatorname{Tr}^{3}(M - \lambda I) + 2 \operatorname{Tr}[(M - \lambda I)^{3}] - 3 \operatorname{Tr}(M - \lambda I) \operatorname{Tr}[(M - \lambda I)^{2}]$$

$$= (N - 3\lambda)^{3} + 2[\operatorname{Tr}(M^{3}) - 3 \operatorname{Tr}(M^{2})\lambda + 3N\lambda^{2} - 3\lambda^{3}] - 3(N - 3\lambda)[\operatorname{Tr}(M^{2}) - 2N\lambda + 3\lambda^{2}]$$

$$= -6\lambda^{3} + 6N\lambda^{2} + \lambda[-3N^{2} + 3 \operatorname{Tr}(M^{2})] + N^{3} + 2 \operatorname{Tr}(M^{3}) - 3N \operatorname{Tr}(M^{2})$$

$$= 6(t + N/3)^{2}(2N/3 - t) + (t + N/3)[-3N^{2} + 3 \operatorname{Tr}(M^{2})] + N^{3} + 2 \operatorname{Tr}(M^{3}) - 3N \operatorname{Tr}(M^{2})$$

$$= -6t^{3} + t[-N^{2} + 3 \operatorname{Tr}(M^{2})] + 4N^{3}/9 - 2N \operatorname{Tr}(M^{2}) + 2 \operatorname{Tr}(M^{3})$$

$$= -6t^{3} + t\left(6\sum_{k < j}(\hat{n}_{j} \cdot \hat{n}_{k})^{2} + 3N - N^{2}\right) + \frac{2}{9}N(N - 3)(2N - 3) - 4(N - 3)\sum_{k < j}(\hat{n}_{j} \cdot \hat{n}_{k})^{2}$$

$$+ 12\sum_{h < i < k}(\hat{n}_{h} \cdot \hat{n}_{j})(\hat{n}_{h} \cdot \hat{n}_{k})(\hat{n}_{j} \cdot \hat{n}_{k}), \tag{A15}$$

and thus we have

$$Det(M - \lambda I) = -t^{3} + t \left(\sum_{k < j} (\hat{n}_{j} \cdot \hat{n}_{k})^{2} - \frac{1}{6} (N - 3)N \right)$$

$$+ \frac{1}{27} N(N - 3)(2N - 3)$$

$$- \frac{2}{3} (N - 3) \sum_{k < j} (\hat{n}_{j} \cdot \hat{n}_{k})^{2}$$

$$+ 2 \sum_{h < j < k} (\hat{n}_{h} \cdot \hat{n}_{j})(\hat{n}_{h} \cdot \hat{n}_{k})(\hat{n}_{j} \cdot \hat{n}_{k}), \quad (A16)$$

which completes the proof of our main result.

APPENDIX B: METHOD OF WEIGHTS

Here, we give a method to compute the incompatibility of the preparation uncertainty which can be used to detect entanglement and steerability. Our technique presented here exploits the structure of appropriate weights between observables, which gives an easy approach to calculate the incompatibility between observables with a large spin number (\geqslant 3). This key trick allows us to go much further beyond the rough estimates of the lower bound of uncertainty relations for all possible quantum states.

First of all, in the calculation of variance for an arbitrary n-dimensional observable M_j , we only need to consider its "effective" part, which belongs to su(n). For any given density matrix ρ and observable with parametrization $M_j = aI + S$, where $S \in su(n)$, we have

$$\operatorname{Tr}(\rho M^2) - [\operatorname{Tr}(\rho M)]^2 = \operatorname{Tr}(\rho S^2) - [\operatorname{Tr}(\rho S)]^2.$$
 (B1)

Thus, $\Delta^2 M = \Delta^2 S$.

Now we only consider the "effective" observable $\{M_j\}$, i.e., Hermitian and traceless matrix. By definitions, the total

uncertainty has the following form,

$$\sum_{i} \Delta^{2} M_{j} = \sum_{i} \operatorname{Tr}(\rho M_{j}^{2}) - \sum_{i} \operatorname{Tr}^{2}(\rho M_{j}),$$
 (B2)

where $\sum_{j} \operatorname{Tr}^{2}(\rho M_{j})$ is a quadratic form and its extreme value can be calculated by its eigenvalues. For the given $\{M_{j}\}$, the functional $\sum_{j} \operatorname{Tr}(\rho M_{j}^{2})$ produces a linear equation. The minimal value of the uncertainty functional $\sum_{j} \Delta^{2} M_{j}$ obtained for the observables $\{M_{j}\}$ becomes difficult to calculate. Actually, by utilizing $\{M_{j}\}$ to detect entanglement and construct EPR-steering criterion, we can not only consider the functional $\sum_{j} \Delta^{2} M_{j}$ but also the weighted functional $\sum_{j} \Delta^{2} p_{j} M_{j}$, where p_{j} is the probability distribution over the set of observables. Compared with the functional $\sum_{j} \Delta^{2} M_{j}$, the weighted sum $\sum_{j} \Delta^{2} p_{j} M_{j}$ may become easy to calculate.

Next, we give some examples of our method: In the case of a three-level system or qutrit, we need the following eight Gell-Mann matrices,

$$\lambda_{1} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_{2} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_{3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_{4} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\lambda_{5} = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_{6} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_{7} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_{8} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \quad (B3)$$

TABLE I. Trace formulas.

Observable	$M = \lambda_1$	$M = \lambda_2$	$M = \lambda_3$	$M = \lambda_4$	$M = \lambda_5$	$M = \lambda_6$	$M = \lambda_7$	$M = \lambda_8$
$Tr(\rho M^2)$	$\frac{2}{3}(1+r_8)$	$\frac{2}{3}(1+r_8)$	$\frac{2}{3}(1+r_8)$	$\frac{2+\sqrt{3}r_3-r_8}{3}$	$\frac{2+\sqrt{3}r_3-r_8}{3}$	$\frac{2-\sqrt{3}r_3-r_8}{3}$	$\frac{2-\sqrt{3}r_3-r_8}{3}$	$\frac{2}{3}(1-r_8)$
$[\operatorname{Tr}(\rho M)]^2$	$\frac{4}{3}r_1^2$	$\frac{4}{3}r_2^2$	$\frac{4}{3}r_3^2$	$\frac{4}{3}r_4^2$	$\frac{4}{3}r_5^2$	$\frac{4}{3}r_6^2$	$\frac{4}{3}r_{7}^{2}$	$\frac{4}{3}r_8^2$

Then, any 3×3 density matrix can be described by the Gell-Mann matrices as

$$\rho = \frac{1}{3}(I + \sqrt{3}r \cdot \lambda), \quad r \in \mathbb{R}^8, \tag{B4}$$

with $\lambda = (\lambda_1, \dots, \lambda_8)$. The non-negativity of ρ demands that r should satisfy the additional inequality [45]

$$|r|^2 = \sum_{j=1}^8 r_j \leqslant 1.$$
 (B5)

The algebraic structure of these matrices is given in Table I.

Note that $\text{Tr}(\rho \lambda_1^2) = \frac{2}{3}(1 + r_8)$ and $\text{Tr}(\rho \lambda_8^2) = \frac{2}{3}(1 - r_8)$ have an opposite coefficient on r_8 . Thus, they reach a constant when sharing the same weight, i.e.,

$$\frac{1}{2}\operatorname{Tr}(\rho\lambda_1^2) + \frac{1}{2}\operatorname{Tr}(\rho\lambda_8^2) = \frac{2}{3},\tag{B6}$$

and hence we also have the following uncertainty relation,

$$\frac{1}{2}\Delta^2\lambda_1 + \frac{1}{2}\Delta^2\lambda_8 \geqslant 0. \tag{B7}$$

Let us notice that, for different weights x and y,

$$x \operatorname{Tr}(\rho \lambda_1^2) + y \operatorname{Tr}(\rho \lambda_8^2) = \frac{2}{3} [x + y + (x - y)r_8],$$
 (B8)

therefore the total minimal of $x\Delta^2\lambda_1 + y\Delta^2\lambda_8$ becomes complicated.

On the other hand, it is impossible to form a constant by weighting the variances $\text{Tr}(\rho \lambda_1^2)$ and $\text{Tr}(\rho \lambda_5^2)$. For this task,

the weight of observable λ_6 might be added,

$$(x, y, 0) \Rightarrow \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right),$$
 (B9)

where x, y, and 0 stand for the weight of $\Delta_{\lambda_1}^2$, $\Delta_{\lambda_5}^2$, and $\Delta_{\lambda_6}^2$, respectively. This leads to the following uncertainty,

$$\frac{1}{3}\Delta^2\lambda_1 + \frac{1}{3}\Delta^2\lambda_5 + \frac{1}{3}\Delta^2\lambda_6 \geqslant \frac{2}{9}.$$
 (B10)

Similarly, we can also get

$$\frac{1}{3}\Delta^2\lambda_2 + \frac{1}{3}\Delta^2\lambda_4 + \frac{1}{3}\Delta^2\lambda_7 \geqslant \frac{2}{9}.$$
 (B11)

Finally, if we use observables $\{M_j\}$ to detect entanglement and EPR steering, some of the observables may increase the difficulty of calculation. For example, consider

$$\{\lambda_1, \lambda_2, \lambda_3, \lambda_5, \lambda_6, \lambda_7, \lambda_8\}$$
 (B12)

with weights $(x_1, x_2, x_3, x_5, x_6, x_7, x_8)$: The total uncertainty may be complicated, while by deleting λ_8 , i.e.,

$$(x_1, x_2, x_3, x_5, x_6, x_7, x_8) \Rightarrow \left(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{3}, \frac{1}{6}, \frac{1}{6}, 0\right), \quad (B13)$$

the possible minimal becomes easy to calculate,

$$\frac{1}{9}\Delta^{2}\lambda_{1} + \frac{1}{9}\Delta^{2}\lambda_{2} + \frac{1}{9}\Delta^{2}\lambda_{3} + \frac{1}{3}\Delta^{2}\lambda_{5} + \frac{1}{6}\Delta^{2}\lambda_{6} + \frac{1}{6}\Delta^{2}\lambda_{7} \geqslant \frac{2}{9}.$$
(B14)

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