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Abstract

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Device-Independent Entanglement Quantification and Related Applications

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We present a general method to quantify both bipartite and multipartite entanglement in a deviceindependent manner, meaning that we put a lower bound on the amount of entanglement present in a system based on the observed data only but independent of any quantum description of the employed devices. Some of the bounds we obtain, such as for the Clauser-Horne-Shimony-Holt Bell inequality or the Svetlichny inequality, are shown to be tight. Besides, device-independent entanglement quantification can serve as a basis for numerous tasks. We show in particular that our method provides a rigorous way to construct dimension witnesses, gives new insights into the question whether bound entangled states can violate a Bell inequality, and can be used to construct device-independent entanglement witnesses involving an arbitrary number of parties.

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Introduction.-Entanglement, undoubtfully the most precious resource of quantum mechanics, has been routinely quantified in many experiments. However, such entanglement statements are generally only valid when a precise quantum description of the employed equipment is available [1]. In many contexts, such a quantum model is not available, in particular for complex biological or condensed matter systems, where one still disputes about the underlying quantum processes or is unsure about the appropriate description of measurements [2,3]. In this case, one can still try to quantify entanglement *exclusively* from the observed classical measurement data, thus independent of any quantum functionality of the interested system. While this may seem impossible at first sight, such methodology is precisely the working principle behind the emergent field of *device-independent* quantum information processing, which started in quantum key distribution [4,5] and device testing [6,7]. However, while it is long known that Bell inequality violations [8] verify entanglement [9], no precise bound on the amount of entanglement is known in the device-independent setting, presumably because nonlocality and entanglement are different resources [10]. Even with a qubit assumption, quantification has so far only been achieved for the simplest experimental scenario [11,12].

In this Letter we present a general framework for various device-independent tasks, notably the quantification of bi- and multipartite entanglement using solely the observed classical data. Incidentally, this provides further results on seemingly unrelated questions in quantum information: First it certifies a necessary minimal dimension of the underlying quantum system and thus provides a rigorous and systematic construction of dimension witnesses [13]. Second, using the negativity [14] as our primary entanglement measure, we obtain new results for the long-standing Peres conjecture [15], which states that no bound entangled

state can violate a Bell inequality. We show that a Bell violation of any known bipartite bound entangled state, or, more precisely, any entangled state with a positive partial transpose (PPT), can at most be very small, if not vanishing, for the simplest classes of Bell inequalities, thus providing circumstantial evidence in favor of this conjecture in the bipartite case. Finally, in the multipartite case our framework additionally facilitates—without resorting to the detection of genuine multipartite non-locality [16]—the construction of device-independent entanglement witnesses (DIEW) for genuine multipartite entanglement [16–18].

Problem definition.—Let us start by considering a bipartite Bell-type experiment where each party can employ different measurement settings x, y with respective outcomes a, b that are sampled from the conditional probability distribution P(a, b|x, y). These data have a quantum representation if there exists a quantum state ρ_{AB} and local measurement operators $M_{a|x}$, $M_{b|y}$ such that P(a, b|x, y) =tr($\rho_{AB}M_{a|x} \otimes M_{b|y}$). In the device-independent paradigm one tries to draw conclusions about ρ_{AB} directly from P(a, b|x, y) without assuming any knowledge of the performed measurements or of the dimension of the underlying state. In order to do so one needs a characterization at the level of P(a, b|x, y) assuming that ρ_{AB} satisfies certain properties. If ρ_{AB} is only required to be a quantum state, we recover the original question leading to Tsirelson's bounds [19–23]. But one can demand ρ_{AB} to fulfill extra constraints, such as being PPT [24], or—with our primary goal in mind-that its entanglement is bounded. This characterization task generalizes naturally to the multipartite case, e.g., to describe if the tripartite distribution P(a, b, c | x, y, z) is quantum, biseparable [16,25], originates from a PPT mixture [26], or has some bounded amount of entanglement.

Our method is a superset characterization, similar to the converging hierarchy proposed by Navascués-Pironio-Acín (NPA) [21–23]. For instance, in the bipartite case we show that a distribution P = P(a, b|x, y) can only originate from a PPT state if a special matrix $\chi[P, u]$, that linearly depends on P and on some unknowns u, satisfies $\chi[P, u] \ge 0$ and $\chi[P, u]^{T_A} \ge 0$. If it is impossible to find such parameters u, then P has no PPT quantum representation. The novel observation which enables us to go beyond NPA is that if one organizes the matrix entries of NPA carefully, the resulting matrix χ can be interpreted as the result of local maps acting on the underlying quantum state. Then this matrix has a clear bipartite structure.

We emphasize that in quantifying entanglement or in characterizing correlations due to extra properties of the quantum state, we need statements that hold for all possible dimensions, measurements and states with the desired property. However, since any measurement operator corresponds to a projector in higher dimensions, we can assume without loss of generality the projection property, i.e., the relation $M_{a|x}M_{a'|x} = \delta_{aa'}M_{a|x}$ for the operators $M_{a|x}$ on system A for all x, a and a'. This follows from Naimark's extension [27] which preserves any entanglement monotone. Also, we shall simultaneously employ the notations $M_{a|x}$ and A_i for measurement operators on system A, likewise for other systems. The set $\{A_i\}$ contains the identity operator $A_0 = 1$ and all but one measurement operator $M_{a|x}$ for each setting. Hence, one has the aforementioned projection property and an identity relation $A_i A_0 = A_0 A_i = A_i$ for all *i*.

Technique.—To solve to the desired characterization problem, we employ results obtained in the studies of matrix of moments for continuous variable systems [28-32] and in the device-independent analysis [20-23].

Let us start with the matrix of moments for the bipartite case and consider first the scenario where the state ρ_{AB} and the measurement operators $M_{a|x}$, $M_{b|y}$ are known. To this scenario we associate two completely positive (CP) *local* maps Λ_A , Λ_B that we apply to the quantum state $\chi[\rho] =$ $\chi[\rho_{AB}]_{\bar{A}\bar{B}} = \Lambda_A \otimes \Lambda_B[\rho_{AB}]$. Here \bar{A} and \bar{B} denote the respective output spaces. Specifically, consider the local map $\Lambda_A[\rho] = \sum K_n \rho K_n^{\dagger}$ where the Kraus operators are given by $K_n = \sum_i |i\rangle_{\bar{A}A} \langle n|A_i$, and $|n\rangle_A$, $|i\rangle_{\bar{A}}$ are orthogonal basis states of \mathcal{H}_A and $\mathcal{H}_{\bar{A}}$, respectively. Using a similar map for *B* one obtains

$$\chi[\rho] = \sum_{ijkl} |ij\rangle_{\bar{A}\bar{B}} \langle kl | \text{tr}[\rho_{AB}A_k^{\dagger}A_i \otimes B_l^{\dagger}B_j].$$
(1)

Thus, the matrix $\chi[\rho]$ is just a matrix of certain expectation values. Since the local maps can also be defined using higher moments, e.g., by choosing Kraus operators $K_n = \sum_{i_1,...,i_\ell} |i_1,...,i_\ell\rangle_{\bar{A}A} \langle n|A_{i_1}A_{i_2}...A_{i_\ell}$, we shall refer to χ as a moment matrix of level ℓ if it contains all ℓ -fold products of A_i . Since both sets $\{A_i\}$, $\{B_j\}$ contain the identity, the trace of the underlying state is a matrix entry that we refer to as $\chi[\rho]_{tr} = tr[\rho]$. Finally, note that by the structure of these local maps we have a couple of important relations: e.g., (i) if $\rho \ge 0$ then $\chi[\rho] \ge 0$, (ii) if $\rho^{T_A} \ge 0$ then $\chi[\rho]^{T_{\bar{A}}} \ge 0$, and (iii) if ρ separable then $\chi[\rho]$ separable. This matrix of moment approach can analogously be defined in the multipartite case.

A device-independent characterization draws a conclusion only from the observed correlations; hence, many of the entries of χ are unknown *a priori*. However, even without this information the matrix $\chi[\rho]$ has a certain structure which follows from known relations that hold independently of state and measurements: (i) A_i , B_j are Hermitian operators, (ii) A_i , B_j satisfies the above mentioned projection property and the identity relation, and (iii) certain entries correspond to the observations $P(a, b|x, y) = \text{tr}(\rho_{AB}M_{a|x} \otimes M_{b|y})$.

Via this partial information we can decompose without loss of generality each matrix of moments $\chi[\rho]$ as

$$\chi[\rho] = \chi[P, u] = \chi^{\text{fix}}(P) + \chi^{\text{open}}(u)$$
$$= \sum_{a,b,x,y} P(a, b|x, y) F_{abxy} + \sum_{v} u_{v} F_{v}, \qquad (2)$$

i.e., into one fixed part that linearly depends on the observed data $\chi^{\text{fix}}(P) = \sum P(a, b|x, y)F_{abxy}$ and into an orthogonal, open part $\chi^{\text{open}}(u) = \sum_{v} u_v F_v$ which would be known only by the knowledge of state and measurements. Here, all operators $F = F^{\dagger}$ are Hermitian. Note that the constraint $\chi[\rho]_{\text{tr}} = \chi[P, u]_{\text{tr}} = 1$ is fulfilled automatically if the probabilities *P* are normalized. We give an example how the relations (1)–(3) provide the form given by Eq. (2) in the Supplemental Material [33].

Connection with the NPA hierarchy.—At this point we like to connect the present technique to that of NPA [21,22], the best known method to characterize quantum correlations. For their method, one can identify a likewise construction $\chi^{\text{NPA}}[\rho] = \Lambda[\rho_{AB}]$, but with Λ being a global CP map which already ensures that if $\rho \ge 0$ then $\chi^{\text{NPA}}[\rho] \ge 0$. If one uses the operator-sum ansatz $\chi^{\text{NPA}}[\rho] = \sum_m L_m \rho L_m^{\dagger}$ where $L_m = \sum_s |s\rangle \langle m|O_s$ with $|m\rangle$, $|s\rangle$ being respective basis states for the in- and output Hilbert spaces, this leads to $\chi^{\text{NPA}}[\rho] = \sum |s\rangle \langle t | \text{tr}[\rho_{AB}O_t^{\dagger}O_s]$. If this operator set $\{O_s\}$ consists of all ℓ -fold products of measurement operators, then imposing the constraint $\chi^{\text{NPA}}[\rho] \ge 0$ corresponds to the ℓ^{NPA} -th step in their hierarchy.

Therefore, a bipartite moment matrix χ of level ℓ as defined above and a 2ℓ -step χ^{NPA} only differ in the ordering of the expectation values and in that certain moments of χ^{NPA} are not included in χ . These similarities are important to relate results about the NPA method χ^{NPA} to the modified moment matrix χ . However, let us stress that χ^{NPA} does not generally admit a bipartite structure.

Applications of technique.—Given the close connection between the present technique and that of NPA, it is clear

that ours can also be used to characterize the set of quantum correlations and hence to compute Tsirelson bounds, i.e., extremal quantum values of a Bell inequality. For instance, for any fixed level ℓ and any given Bell expression $I \cdot P = \sum I_{abxy} P(a, b | x, y)$, an upper bound to the Tsirelson bound can be obtained by solving max $\{I \cdot P | \chi[\rho] = \chi[P, u] \ge 0\}$ as a semidefinite program [34]. Henceforth, let us focus on the novel applications that stem from the current technique.

In comparison with NPA the advantage of the additional bipartite structure $\chi = \chi_{\bar{A}\bar{B}}$ is that one can now easily incorporate further constraints. For instance, one could ask for a similar Tsirelson bound if the underlying state is PPT by including the constraint $\chi[\rho]^{T_{\bar{A}}} \ge 0$,

$$\max_{P,u} I \cdot P \tag{3}$$

s.t.
$$\chi[\rho] = \chi[P, u] \ge 0$$
, $\chi[\rho]^{T_{\bar{A}}} \ge 0$, $\chi[\rho]_{tr} = 1$.

By this method one obtains an upper bound to the true PPT Tsirelson bound, which converges to the related commutative bound in the limit of large levels ℓ , see Supplemental Material [33] for details.

Next, let us show how to estimate the negativity [14], defined via the sum of negative eigenvalues λ_i of the partially transposed state as $N[\rho_{AB}] = \sum_{\lambda_i < 0} |\lambda_i(\rho_{AB}^{T_A})|$. In the following we employ its variational form which reads as $N[\rho_{AB}] = \min\{tr[\sigma_-]|\rho_{AB} = \sigma_+ - \sigma_-, \sigma_{\pm}^{T_A} \ge 0\}$. Using the properties of the moment matrix, one can readily optimize over a larger set: The constraint $\rho = \sigma_+ - \sigma_-$ is relaxed by $\chi[\rho] = \chi[\sigma_+] - \chi[\sigma_-]$, while $\sigma_{\pm}^{T_A} \ge 0$ translates to $\chi[\sigma_{\pm}]^{T_A} \ge 0$. If one observes a certain violation of a Bell inequality $I \cdot P = v$, a lower bound on the negativity of ρ_{AB} compatible with this observation is given by

$$\min_{P,u,P_{\pm},u_{\pm}} \chi[\sigma_{-}]_{\rm tr} \tag{4}$$

s.t.
$$\chi[\rho] = \chi[P, u] = \chi[\sigma_+] - \chi[\sigma_-] \ge 0, \quad \chi[\rho]_{tr} = 1,$$

 $\chi[\sigma_\pm]^{T_{\tilde{A}}} = \chi[P_\pm, u_\pm]^{T_{\tilde{A}}} \ge 0, \quad I \cdot P = v.$

Furthermore, since the negativity of any $\mathbb{C}^d \otimes \mathbb{C}^D$ state is at most $N_{\max}^d = (d-1)/2$ (for $d \leq D$), a lower bound on the negativity certifies also a minimal state space dimension. The bound of a dimension witness [13], i.e., the maximal value of a Bell inequality for states with minimal local dimension upper bounded by d, can be constructed by an optimization analogous to Eq. (4) but with the expression $I \cdot P$ now appearing in the objective function, while the dimension restriction is enforced by the constraint $\chi[\sigma_{-}]_{tr} \leq N_{\max}^d$.

At this point we like to stress that these optimization problems admit a natural generalization to the multipartite scenario using PPT mixtures (which include biseparable states) and the genuine negativity as a measure for genuine multiparticle entanglement [26]. Further details and the explicit programs are given in Supplemental Material [33]. *Example I: CHSH.*—Let us start with the Clauser-Horne-Shimony-Holt (CHSH) inequality [35], where each party has two possible settings $x, y \in \{1, 2\}$ yielding binary outcomes a, b. Using correlation terms $\langle X_x Y_y \rangle =$ $P(a = b|x, y) - P(a \neq b|x, y)$, the inequality $I_{CHSH} =$ $\langle X_1 Y_1 \rangle + \langle X_1 Y_2 \rangle + \langle X_2 Y_1 \rangle - \langle X_2 Y_2 \rangle \leq 2$ holds for any local hidden-variable model (LHV), while quantum mechanics allows a maximum of $I_{CHSH}^{max} = 2\sqrt{2}$. Since every separable state fulfills the LHV bound [9], any violation $I_{CHSH} > 2$ signals entanglement of the underlying quantum state ρ_{AB} . By solving Eq. (4) we can now provide a quantitative statement in terms of the minimal negativity that the underlying state ρ_{AB} must possess. Specifically, the numerical result leads to the sharp bound

$$N[\rho_{AB}|I_{\text{CHSH}} = v] \ge (v-2)/(4\sqrt{2}-4).$$
(5)

The resulting plot and a more detailed discussion, also about the other examples, can be found in Supplemental Material [33]. Note that this recovers the known result that PPT states must necessarily satisfy the CHSH inequality [36].

Example II: Dimension witness.—As a second example, we consider the Bell inequality $I_{3322} \leq 0$ [37,38], where each party can perform three possible dichotomic measurements as indicated by the subscripts. For a violation of $0 \leq v \leq 0.25$, the numerical solution of Eq. (4) gives $N[\rho_{AB}|I_{3322} = v] \geq 2v$ and a two-qubit Bell state can indeed reach a violation of $I_{3322} = 0.25$ [38]. However, the maximum possible quantum violation is given by $I_{3322}^{max} \leq 0.25088$ and there exist infinite-dimensional states which can asymptotically reach this value [39]. From Fig. 1, we see more closely that if $I_{3322} > 0.25$ the negativity bound satisfies $N[\rho_{AB}] > 1/2$, which is achievable only with local Hilbert space dimension $d \geq 3$. Hence, $I_{3322} \leq 0.25$ serves as a dimension witness for qutrits. In a similar way we investigated the very first Bell



FIG. 1 (color online). Negativity bounds for violations close to the maximum of the Bell inequality I_{3322} [37,38] obtained by solving Eq. (4) for different levels of the moment matrix. Note that violations with v > 0.25 require a negativity of $N[\rho_{AB}] > 1/2$ and thus at least a two-qutrit state.

TABLE I. Upper bounds on the maximal possible violation by PPT states for different Bell inequalities computed via Eq. (3). All the other four dichotomic setting Bell inequalities investigated have a PPT Tsirelson bound which is already within the respective LHV bound by less than 10^{-6} . Further specifications: ℓ labels levels of the matrix of moment, "Matrix size" refers to the dimension of the moment matrix. The last inequality corresponds to the tripartite case for states which are PPT for all bipartitions. The precision is at least 10^{-7} .

Bell inequality	PPT Tsirelson bound	l	Matrix size
$I_{\rm CHSH} \le 2 \ [35]$	2	1	$3^2 \times 3^2$
$I_{3322} \le 0$ [38]	0	2	$10^{2} \times 10^{2}$
$I_{2233} \le 0$ [38]	$\leq 1.3559 \times 10^{-3}$	3+	$45^{2} \times 45^{2}$
$A_6 \le 0$ [42]	\leq 7.6754 \times 10 ⁻⁶	2 +	$31^2 \times 31^2$
$I_{4422}^3 \leq 0$ [42]	$\leq 2.8531 \times 10^{-4}$	2 +	$27^{2} \times 27^{2}$
$I_{S5} \leq 3$ [37]	≤3.0187	3	$7^{3} \times 7^{3}$

inequality used as a dimension witness [13], namely, $I_{2233} \leq 0$ [38,40,41], and confirm that violations larger than $v = 1/\sqrt{2} - 1/2 \approx 0.2071$ require at least qutrits this certifies the heuristic qubit bound of I_{2233} [13].

Example III: PPT Tsirelson bound.—As a third example of the application of our techniques, we have computed upper bound on the PPT Tsirelson bound for the above Bell inequalities and 175 facet-defining Bell inequalities involving four dichotomic measurement settings per party [42–44]. Interestingly, our results show that for the majority of these inequalities, the maximal quantum violation allowed by all PPT entangled states is vanishing within numerical precision, and, hence, unable to provide a counterexample to the bipartite Peres conjecture; cf. Table I and Supplemental Material [33] for details.

Multipartite case.--We also considered examples involving more than two parties, where one is typically interested to verify genuine multipartite entanglement. This strongest form of multiparticle entanglement can be detected from observed correlations alone by violating a DIEW [16]. For device-independent entanglement quantification, we investigated-by a method analogous to the bipartite case-the minimal amount of genuine negativity [26] needed to violate the DIEWs I_{32} and I_{33} , where each party has respectively two or three dichotomic measurements [16,45]. Since I_{32} is the Svetlichny inequality [46], its violation also demonstrates genuine multipartite nonlocality. From the bounds we computed, again tight for the Svetlichny case (see Supplemental Material [33]), we can also obtain information about the type of entanglement responsible for given violations, in similar spirit to Ref. [47]. For instance, since the genuine negativity of any state of the three-qubit W-class [48] is bounded by $\sqrt{2/3}$, one verifies that violations close to the maximum of these DIEWs can never be achieved by such type of entanglement. Moreover, our bounds show that these DIEWs can never be violated by states which are PPT mixtures [26]. Using similar arguments as presented in Ref. [18], this result can even be extended to the *n*-partite witnesses I_{n2} and I_{n3} . This suggests that, apart from a quantification, the generalization of PPT Tsirelson bounds to the multipartite case provides a tractable way to approximate the set of biseparable quantum correlations in the presence of more than three parties [16]. Indeed, this approximation not only works well for the two families of *n*-partite DIEWs I_{n2} , I_{n3} , but also for a large number of symmetric 4-partite DIEWs involving two dichotomic measurements [49].

Finally, there are also other questions for the multipartite case. At last we computed the maximal violation of the tripartite Bell inequality $I_{S5} \leq 3$ [37] for states which are PPT for all bipartitions. We find that it is bounded by 3.0187, which shows that the example of Ref. [50], optimally violates the tripartite Peres conjecture via this inequality, cf. Table I.

Conclusion.—We have presented a versatile tool to quantify entanglement in the bi- and multipartite case directly from the observed measurement results, thus irrespective of any quantum functionality of the employed devices. This framework offers great practical benefit in experiments since its statements are robust against any kind of systematic errors in the assumed quantum model and involves minimal assumptions. Moreover such a quantification provides additional applications: It yields information about the underlying state space dimension or the type of entanglement involved in the multipartite case. Furthermore, our tool allows for a systematic investigation into the long-standing Peres conjecture, and the computation of device-independent entanglement witness for genuine multipartite entanglement.

For future work, we believe that our method can be extended to bound, in a device-independent manner, other entanglement measures. Clearly, it will also be interesting to investigate how our technique can be used in conjunction with other separability criteria, or applied in the closely related steering [51] (with the partial information step only applied to one-side) or sequential measurement scenarios [52].

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