Bound Entanglement from Randomized Measurements

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If only limited control over a multiparticle quantum system is available, a viable method to characterize correlations is to perform random measurements and consider the moments of the resulting probability distribution. We present systematic methods to analyze the different forms of entanglement with these moments in an optimized manner. First, we find the optimal criteria for different forms of multiparticle entanglement in three-qubit systems using the second moments of randomized measurements. Second, we present the optimal inequalities if entanglement in a bipartition of a multiqubit system shall be analyzed in terms of these moments. Finally, for higher-dimensional two-particle systems and higher moments, we provide criteria that are able to characterize various examples of bound entangled states, showing that detection of such states is possible in this framework.

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Introduction.-With the current development of experimental quantum technologies, larger quantum systems with more and more particles become available, but controlling and analyzing these systems is complicated. In fact, due to the exponentially increasing dimension of the underlying Hilbert space, a complete characterization of the quantum states or quantum dynamics is quickly out of reach. A key idea for analyzing large quantum systems is therefore to perform random measurements or operations, and to characterize the global quantum system with the help of the observed statistics. Examples are procedures like randomized benchmarking for the analysis of quantum gates [1,2], certain methods for estimating the fidelity of quantum states [3], or various proposals to perform variants of state tomography using random measurements [4-7].

It was noted early that randomized measurements could also be used to study quantum correlations [8–10]. The original motivation came from the situation where two parties, typically called Alice and Bob, share a quantum state but no common reference frame. This situation has been discussed in a variety of settings in quantum information processing [11–14]. Although the determination of the entire quantum state is impossible in this setting, it may still be analyzed along the following lines. Alice and Bob perform separate measurements, denoted by M_A and M_B , and rotate them arbitrarily. That is, they evaluate an expression of the form

$$\langle M_A \otimes M_B \rangle_{U_A \otimes U_B} = \operatorname{tr}[\varrho_{AB}(U_A M_A U_A^{\dagger}) \otimes (U_B M_B U_B^{\dagger})],$$
(1)

which, of course, depends on the chosen unitary $U_A \otimes U_B$. The prime idea is to sample random unitaries and consider the resulting probability distribution of $\langle M_A \otimes M_B \rangle_{U_A \otimes U_B}$. This probability distribution contains valuable information about the state, and the distribution may be characterized by its moments

$$\mathcal{R}_{AB}^{(r)} = \int dU_A \int dU_B [\langle M_A \otimes M_B \rangle_{U_A \otimes U_B}]^r, \quad (2)$$

where the unitaries are typically chosen according to the Haar distribution. Clearly, similar moments can be defined for multiparticle systems.

In recent years, several works proceeded in this direction. One research line has been started from the estimation of the state's purity [15], and then protocols for measuring entanglement via Rényi entropies have been presented [16] and experimentally implemented [17]. Very recently, ideas to estimate the entanglement criterion of the positivity of the partial transpose (PPT) [18,19] have been introduced [20,21]. Another research line characterized the relation of the second moments [22,23] $\mathcal{R}_{AB}^{(2)}$ and those of the marginals [24] to entanglement. Recently, higher moments have been used to characterize multiparticle entanglement [25,26], and quantum designs have been shown to allow for a simplified implementation, because the integral in Eq. (2) can be replaced by finite sums [25,27,28].

Still, the present results along the above research lines are incomplete in several respects. First, although many entanglement criteria have been presented, their optimality is not clear. It would be desirable to use the information obtained by randomized measurements most efficiently. Second, the known results from randomized measurements allow one to detect highly entangled states only, e.g., states that are close to pure states. For a long-range impact of the research program, however, it is vital that weakly entangled states (e.g., the ones that cannot be detected by the PPT criterion) can also be analyzed.

The goal of this Letter is to generalize the existing approaches in two directions: First, we will systematically consider the moments of the measurement results when only some of the parties measure. That is, we evaluate the expressions in Eqs. (1) and (2) for the special case of $M_A = 1$ or $M_B = 1$, and we call these quantities the reduced moments $\mathcal{R}_B^{(r)}$ and $\mathcal{R}_A^{(r)}$. Note that this case effectively corresponds to discarding the measurements of Alice for $\mathcal{R}_B^{(r)}$ (respectively, Bob for $\mathcal{R}_A^{(r)}$) such that the reduced moments can directly be evaluated from the data taken for measuring $\mathcal{R}_{AB}^{(r)}$. As we will show, in terms of these reduced moments, improved entanglement criteria can be designed that are optimal in the sense that if a quantum state is not detected by them, then there is also a separable state compatible with the data.

Second, we present a systematic approach to characterize high-dimensional systems with higher moments $\mathcal{R}_{AB}^{(r)}$. We show how previously known entanglement criteria [29–31] can be formulated in terms of moments. With this, we demonstrate that bound entanglement, which is a weak form of entanglement that cannot be used for entanglement distillation and is not detectable by the PPT criterion, can be also characterized in a reference-frame independent manner. This shows that the approach of randomized measurements is powerful enough to characterize the rich plethora of entanglement phenomena.

Multiparticle correlations for three qubits.—For three qubits, the measurements M_A , M_B , and M_C may, without loss of generality, be taken as the Pauli-Z matrix σ_3 . If we consider the full or reduced second moments $\mathcal{R}^{(2)}$, the analysis is simplified by the fact that each integral over U(2) in Eq. (2) can be replaced by sums over the four Pauli matrices σ_0 , σ_1 , σ_2 , and σ_3 . This is because the Pauli matrices form a unitary two-design, meaning that averages of polynomials of degree two or less yield identical results [25,32].

Accordingly, the moments are directly related to the Bloch decomposition of the three-qubit state q_{ABC} . Recall that any three-qubit state can be written as

$$\varrho_{ABC} = \frac{1}{8} \sum_{i,j,k=0}^{3} \alpha_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k, \qquad (3)$$

where $\sigma_0 = 1$ denotes the identity matrix. The full and reduced second moments can simply be expressed in terms of the coefficients α_{ijk} , and they read



FIG. 1. Geometry of the three-qubit state space in terms of the second moments of random measurements or sector lengths. The total polytope is the set of all states, characterized by the inequalities $A_k \ge 0$, $A_1 - A_2 + A_3 \le 1$, $A_2 \le 3$, and $A_1 + A_2 \le 3(1 + A_3)$ [36]. The fully separable states are contained in the blue polytope, obeying the additional constraint in Eq. (6) in observation 1. States that are biseparable for some partitions are contained in the union of the green and blue polytopes, characterized by the additional equation [Eq. (7)] from observation 2. In fact, for any point in the green and blue areas, there is a biseparable state with the corresponding second moments. The yellow area corresponds to the states violating the best previously known criterion for biseparable states, $A_3 \le 3$ [33–36]. Thus, the red area marks the improvement of the criterion in observation 2 compared with previous results.

$$\mathcal{R}_{ABC}^{(2)} = \frac{1}{27} \sum_{i,j,k=1}^{3} \alpha_{ijk}^{2}, \ \mathcal{R}_{AB}^{(2)} = \frac{1}{9} \sum_{i,j=1}^{3} \alpha_{ij0}^{2}, \ \mathcal{R}_{A}^{(2)} = \frac{1}{3} \sum_{i=1}^{3} \alpha_{i00}^{2},$$
(4)

and similarly for the reduced moments on other parts of the three-particle system.

Sums of this form have already been considered under the concept of sector lengths [33–37] and multiparticle concurrences [38,39]. More precisely, the notion of sector lengths captures the magnitude of the one-, two-, and three-body correlations in the state ρ_{ABC} , where the one- and two-body correlations are averaged over all one- and two-particle reduced states. That is, the sector lengths A_k are given by $A_1 = 3(\mathcal{R}_A^{(2)} + \mathcal{R}_B^{(2)} + \mathcal{R}_C^{(2)})$, $A_2 = 9(\mathcal{R}_{AB}^{(2)} + \mathcal{R}_{AC}^{(2)} + \mathcal{R}_{BC}^{(2)})$, and $A_3 = 27\mathcal{R}_{ABC}^{(2)}$. Most importantly, the set of all three-qubit states forms a polytope in the space of the sector lengths, which has recently been fully characterized [36]; see also Fig. 1.

To proceed, recall that a state is fully separable if it can be written as

$$\varrho_{\rm fs} = \sum_{k} p_k \varrho_k^A \otimes \varrho_k^B \otimes \varrho_k^C, \tag{5}$$

where the p_k form a probability distribution. Now, we can formulate the first main result of this Letter.

Observation 1.—Any fully separable three-qubit state obeys

$$A_2 + 3A_3 \le 3 + A_1 \tag{6}$$

or, equivalently,

$$3(\mathcal{R}_{AB}^{(2)} + \mathcal{R}_{AC}^{(2)} + \mathcal{R}_{BC}^{(2)}) + 27\mathcal{R}_{ABC}^{(2)} \le 1 + \mathcal{R}_{A}^{(2)} + \mathcal{R}_{B}^{(2)} + \mathcal{R}_{C}^{(2)}.$$

This is the optimal linear criterion in the sense that any other linear criterion for the A_i detects strictly fewer states.

The proof of this observation, including possible generalizations to higher-dimensional systems, is given in Appendix A in the Supplemental Material [40], and the geometrical interpretation is displayed in Fig. 1.

Violation of Eq. (6) implies that the state contains some entanglement, but it does not mean that all three particles are entangled. Indeed, an entangled state may still be separable with respect to some bipartition. For instance, if we consider the bipartition A|BC, a state separable with respect to this bipartition can be written as

$$arrho_{A|BC} = \sum_k q_k^A arrho_k^A \otimes arrho_k^{BC},$$

where the q_k^A form a probability distribution, and ϱ_k^{BC} may be entangled. Similarly, one can define biseparable states with respect to the two other bipartitions as $\varrho_{B|AC}$ and $\varrho_{C|AB}$. For these states, we can formulate the following:

Observation 2.—Any three-qubit state that is separable with respect to some bipartition obeys

$$A_2 + A_3 \le 3(1 + A_1) \tag{7}$$

or, equivalently,

$$3(\mathcal{R}_{AB}^{(2)} + \mathcal{R}_{AC}^{(2)} + \mathcal{R}_{BC}^{(2)}) + 9\mathcal{R}_{ABC}^{(2)} \le 1 + 3(\mathcal{R}_{A}^{(2)} + \mathcal{R}_{B}^{(2)} + \mathcal{R}_{C}^{(2)}).$$

This is the optimal criterion in the sense that if the three A_i obey the inequality, then for any bipartition, there is a separable state compatible with them.

Again, the proof and the generalizations to higher dimensions are given in Appendix A [40], and the geometry is displayed in Fig. 1. We add that we have strong numerical evidence that Eq. (7) also holds for mixtures of biseparable states with respect to different partitions, i.e., states of the form $\rho_{\rm bs} = p_A \rho_{A|BC} + p_B \rho_{B|AC} + p_C \rho_{C|AB}$, where the p_A , p_B , and p_C form convex weights. Nevertheless, we leave this as a conjecture for further study. More detailed information on the numerical methods used can be found in Appendix D [40].

Our two observations show that not only the three-body second moment $\mathcal{R}_{ABC}^{(2)}$ but also the one- and two-body reduced moments such as $\mathcal{R}_{AB}^{(2)}$ and $\mathcal{R}_{A}^{(2)}$ can be useful for entanglement detection. In fact, their linear combinations allow us to detect entangled states more efficiently than existing criteria [33–36]; see also Appendix A [40]. In particular, as shown in the Appendix, Eq. (7) can detect multipartite entanglement for mixtures of Greenberger-Horne-Zeilinger (GHZ) states and W states (i.e., $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$, $|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$, even if two other important entanglement measures, namely the three-tangle and bipartite entanglement in the reduced subsystems vanish simultaneously [62].

Optimal criteria for general bipartitions.—In many realistic scenarios, it is sufficient to detect entanglement across some fixed bipartition $I|\bar{I}$ of the multiparticle system. For this task, second moments of randomized measurements can be used as well: Performing random measurements at each qubit and considering the second moments allow one to generalize the moments in Eq. (4) for the given number of qubits. In turn, these moments allow one to determine the quantities $tr(q_I^2)$, $tr(q_{\bar{I}}^2)$, and $tr(q^2)$ for the reduced states of the bipartition and the global state. This approach has recently been used in an experiment [17] where entanglement criteria with the second-order Rényi entropy $S_2(\varrho_X) = -\log_2 \operatorname{tr}(\varrho_X^2)$ were employed. The entropic criteria for separable states read $S_2(q_X) \leq$ $S_2(\rho)$ for $X = I, \overline{I}$; if this is violated, then ρ is entangled [16,63,64].

Using our methods, we can show that this approach is optimal. To formulate the result, we assume that both sides of the bipartition have the same number of qubits. Then, we recall that any bipartite state can be written as

$$\varrho_{AB} = \frac{1}{d^2} \sum_{i,j=0}^{d^2-1} t_{ij} \lambda_i \otimes \lambda_j, \qquad (8)$$

where $\lambda_0 = 1$ denotes the identity matrix, and λ_i are the Gell-Mann matrices [65,66]. This is the decomposition of ρ_{AB} using the basis of Hermitian, orthogonal, and traceless matrices; i.e., $\lambda_i = \lambda_i^{\dagger}$, $\operatorname{tr}[\lambda_i \lambda_j] = d\delta_{ij}$, and $\operatorname{tr}[\lambda_i] = 0$ for i > 0. These properties are the natural extensions of Pauli matrices for SU(2) to SU(d), which are used in particle physics [67]. The quantities of interest are

$$A_2 = \sum_{i,j=1}^{d^2-1} t_{ij}^2, \qquad A_1^A = \sum_{i=1}^{d^2-1} t_{i0}^2, \qquad A_1^B = \sum_{i=1}^{d^2-1} t_{0i}^2.$$
(9)

We also define $A_1 = A_1^A + A_1^B$, which allows us to recover the purities via $tr(\varrho_{AB}^2) = (1 + A_1 + A_2)/d^2$ and $tr(\varrho_A^2) = (1 + A_1^A)/d$. It is interesting that, although the λ_i are *not* directly linked to a quantum design, the quantities A_1^A, A_1^B , and A_2 are also second moments of a measurement of the observables λ_i in random bases. The proof follows from a slight extension of the arguments given in Ref. [23]; see Appendix B [40]. This opens another possibility for an experimental implementation besides making randomized Pauli measurements on all the qubits individually. Now, we can formulate the following:

Observation 3.—Any two-qudit separable state obeys the relation

$$A_2 \le d - 1 + (d - 1)A_1^A - A_1^B, \tag{10}$$

as well as the analogous one with parties *A* and *B* exchanged. This is equivalent to the criterion $S_2(\varrho_X) \leq S_2(\varrho_{AB})$ for $X \in \{A, B\}$. This criterion is optimal, in the sense that if the inequality holds for A_1^A , A_1^B , and A_2 , then there is a separable state compatible with these values.

The criterion itself was established before, and so we only have to prove the optimality statement. This is done in Appendix A [40], where we explicitly construct the polytope of all admissible values of A_1^A , A_1^B , and A_2 for general and separable states in any dimension. The unfortunate consequence of the optimality statement is that any PPT entanglement cannot be detected by the quantities A_1^A , A_1^B , and A_2 because the entropic criterion is strictly weaker than the PPT criterion [68]. In the following, we will overcome this obstacle by developing a general criterion for entanglement using higher moments of randomized measurements.

Higher-dimensional systems.—In higher-dimensional systems, different forms of entanglement exist, e.g., entanglement of different dimensionality [69,70] or bound entanglement [71–74]. The previously known criteria for randomized measurements face serious problems in this scenario. First, criteria using purities, such as observation 3, can only characterize states that violate the PPT criterion. and hence miss the bound entanglement. Second, although the notion of randomized measurements as defined in Eqs. (1) and (2) is independent of the dimension, many results for qubits employ the concept of a Bloch sphere, which is not available for higher dimensions, where not all observables are equivalent under randomized unitaries. Reference [23] showed that some results for qubits are also valid for higher dimensions as long as only second moments are considered, but these connections are definitely not valid for higher moments.

To overcome these problems, we first note that a general observable is characterized by its eigenvectors, determining the probabilities of the outcomes, and the eigenvalues, corresponding to the observed values. For computing the moments as in Eq. (2), the eigenvectors do not matter due to the averaging over all unitaries. The eigenvalues are relevant, but they may be altered in classical postprocessing: Once the frequencies of the outcomes are recorded, one can calculate the moments in Eq. (2) for different assignments of values to the outcomes.

So, the question arises of whether one can choose the eigenvalues of an observable in a way that the moments in Eq. (2) are easily tractable. For instance, it would be desirable to write them as averages over a high-dimensional sphere (the so-called pseudo-Bloch sphere). The reason is that several entanglement criteria, such as the computable cross norm or realignment criterion [29,30] and the de Vicente (dV) criterion [31], also make use of a pseudo-Bloch sphere [75]. Surprisingly, the desired eigenvalues can always be found:

Observation 4.—Consider an arbitrary observable in a higher-dimensional system. Then, one can change its eigenvalues such that, for the resulting observable M_d , the second and fourth moments $\mathcal{R}_{AB}^{(r)}$ in the sense of Eq. (2) equal (up to a factor) a moment $\mathcal{S}_{AB}^{(r)}$ that is taken by an integral over a generalized pseudo-Bloch sphere. That is, $\mathcal{S}_{AB}^{(r)}$ is given by

$$\mathcal{S}_{AB}^{(r)} = N \int d\boldsymbol{\alpha}_1 \int d\boldsymbol{\alpha}_2 [\operatorname{tr}(\varrho_{AB}\boldsymbol{\alpha}_1 \cdot \boldsymbol{\lambda} \otimes \boldsymbol{\alpha}_2 \cdot \boldsymbol{\lambda})]^r, \quad (11)$$

where α_i denote $(d^2 - 1)$ -dimensional unit real vectors uniformly distributed from the pseudo-Bloch sphere, and $\lambda = (\lambda_1, \lambda_2, ..., \lambda_{d^2-1})$ is the vector of the Gell-Mann matrices. Furthermore, *N* is a normalization factor.

The proof and the detailed form of M_d are given in Appendix B [40]. To give a simple example, for d = 3, one may measure the standard spin measurement J_z and assign the values α_+/γ , α_-/γ , and $2\beta/\gamma$ instead of the standard values ± 1 and 0 to the three possible outcomes, where $\alpha_{\pm} = \pm 3 - \beta$, $\beta = -\sqrt{7 + 2\sqrt{15}}$, and $\gamma = 2\sqrt{5 + \sqrt{15}}$. Note that the resulting observable is also traceless.

It remains to formulate separability criteria in terms of the second and fourth moments $S_{AB}^{(r)}$. For that, we employ the dV criterion [31], details of the calculations are given in Appendix B [40]. From these results, it also follows that the dV criterion can be evaluated via randomized measurements for all dimensions. First, it turns out that $\mathcal{S}_{AB}^{(2)}$ and $\mathcal{S}_{AB}^{(4)}$ can, for any dimension, be simply expressed as polynomial functions of the subset of the two-body correlation coefficients t_{ij} with $1 \le i, j \le d^2 - 1$ in Eq. (8), where we also call this submatrix T_s . Second, the moments $\mathcal{S}_{AB}^{(r)}$ are by definition invariant under orthogonal transformations of the matrix T_s . On the other hand, the dV criterion reads that two-qudit separable states obey $||T_s||_{tr} \leq d-1$, and this is also invariant under the named orthogonal transformations. Third, for a fixed value of the second moment $S_{AB}^{(2)}$, we can maximize and minimize the fourth moment $S_{AB}^{(4)}$ under the constraint $||T_s||_{tr} \le d - 1$. This task is greatly simplified by orthogonal invariance; in fact, we can assume T_s to be diagonal. This leads to simple, piecewise algebraic separability conditions for arbitrary dimensions d.

The results for d = 3 are shown in Fig. 2. The outlined procedure gives an area that contains all values of $S_{AB}^{(2)}$



FIG. 2. Entanglement criterion based on second and fourth moments of randomized measurements for $3 \otimes 3$ systems. Separable states are contained in the light-blue area, according to the discussion in the main text. Several bound entangled states (denoted by colored symbols) are outside, meaning that their entanglement can be detected with the methods developed in this Letter. For comparison, we also indicate a lower bound on the fourth moment for PPT states, obtained by numerical optimization, as well as a bound for general states. Further details, such as the forms of the states, are given in Appendix C. Information on the numerical methods is found in Appendix D [40].

and $S_{AB}^{(4)}$ for separable states. Most importantly, various bound entangled states can be detected [76–79]. Also, for d = 4, bound entanglement can be detected; details are given in Appendix C [40].

Conclusion.—We have developed methods for characterizing quantum correlations using randomized measurements. On the one hand, our approach led to optimal criteria for different forms of entanglement using the second moments of the randomized measurements. On the other hand, we have shown that using fourth moments of randomized measurement detection of bound entanglement as a weak form of entanglement is possible. This opens a new perspective for developing the approach further because all previous entanglement criteria were only suited for highly entangled states.

There are several directions for further research. First, on a more technical level, the employed separability criterion [31] can be derived from an approach toward entanglement using covariance matrices [80]. Connecting randomized measurements to this approach will automatically lead to further results, e.g., on the quantification of entanglement [81]. Second, for experimental studies of the criteria presented in this Letter, a scheme for the statistical analysis of finite data (e.g., using the Hoeffding inequality or other large deviation bounds) is needed. Finally, our results encourage development of the characterization of other quantum properties using randomized measurements, such as spin squeezing or the quantum Fisher information in metrology.

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