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Correlated multipartite quantum states

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We investigate quantum states that possess both maximum entanglement and maximum discord between the pertinent parties. Since entanglement (discord) is defined only for bipartite (two-qubit) systems, we use an appropriate sum over all bipartitions as the associated measure. The ensuing definition—not new for entanglement—is thus extended here to quantum discord. Also, additional dimensions within the parties are considered (*qudits*). We also discuss quantum correlations that induce Mermin's Bell-inequality violation for all multiqubit systems. One finds some differences when quantum mechanics is defined over the field of real or of complex numbers.

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I. INTRODUCTION

The concept of quantum correlation for multipartite systems is intimately related to the mathematical structure of quantum mechanics, as a direct consequence of the linear character of tensor-product Hilbert spaces [1,2]. It is the aim of the present work to regard multipartite quantum correlations [2] from three standpoints: those of (1) quantum entanglement, (2) quantum discord, and (3) quantum correlations responsible for Mermin's Bell-inequality violation, here abbreviated withyout distinction as either Mermin-Ardehali-Belinskii-Klyshko (MABK) violation or MABK correlations [3].

Remember that such violation by decohered Greenberger-Horne-Zeilimger (GHZ) states grows exponentially with the number of particles N, despite the fact that both entanglement and nonlocal content decay exponentially. This was the first spectacular demonstration of the fact that there is no limit to the amount by which the quantum-mechanical correlations can exceed the limits imposed by a Bell inequality [2].

Maximally entangled states of up to $N = 6$ qubits will be reconsidered here in the light of their tensor-product structure, basic for discussing the nature of truly multipartite correlations. Multiqudit states will also be explored. Our description addresses entanglement in qudit systems of several parties. In addition, we will assess how different measures of quantum correlations relate to each other, advancing interesting connections between them. Lastly, we introduce an original state of $N = 8$ qubits with maximal multipartite quantum discord.

The paper is organized as follows. In Sec. II we study maximally entangled states for $N = 3,4,\ldots,8$ qubits. Section III is devoted to obtaining maximally entangled states for systems of *qudits*, and comparing them with their corresponding qubit counterparts. Section IV makes use of quantum discord in order to find a multipartite qubit system that maximizes it. Section V compares all correlation measures by individually studying how they evolve as the number of parties increases. Finally, some conclusions are drawn in Sec. VI.

II. MAXIMALLY ENTANGLED STATES OF MULTIQUBIT SYSTEMS

A. Preliminaries

A convenient basis for dealing with correlated multipartite states of N qubits is given by

$$|\Psi^{\pm}_{j,N}\rangle = (|j\rangle \pm |2^N - 1 - j\rangle)/\sqrt{2}. \tag{1}$$

Notice that these states maximally violate the generalized MABK Bell inequality [4]. For $N = 3$ qubits, the maximally entangled state is given by the usual GHZ state $|\mathrm{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$. This instance will be the only one for which maximum entanglement and maximum MABK violation are provided by the same state. For $N = 4$ qubits, the state discovered by Higuchi and Sudbery [5], given by

$$|\Phi_4\rangle = \frac{1}{\sqrt{3}}[|\Psi^{+}_{3,4}\rangle + \omega|\Psi^{+}_{6,4}\rangle + \omega^2|\Psi^{+}_{5,4}\rangle] \tag{2}$$

with $\omega = -\frac{1}{2} + \frac{\sqrt{3}}{2}i$, is the one which possesses maximum entanglement ($9.3773 \ln 2$) as defined by the von Neumann measure

$$S_{\mathrm{vN}} = \sum_i -\mathrm{Tr}[\rho_i \ln \rho_i]. \tag{3}$$

For this entanglement measure to be optimal, the corresponding state must possess complex expansion coefficients. In addition, the quantum discord (QD) is not equal to zero for state (2). The MABK Bell-inequality maximal violation is given by

$$\mathrm{MABK}^{\max}_N \equiv \max_{\mathbf{a}_j,\mathbf{b}_j} \mathrm{Tr}(\rho B_N). \tag{4}$$

In the complex case of four qubits, $\mathrm{MABK}^{\max}_4 = 2.177\,32$, 38% of the maximum possible violation.

For $N = 5$ qubits, Brown *et al.* [6] proposed a state which is shown to possess the maximum entanglement as given by (3). This state of five qubits is of the form

$$|\Phi_5\rangle = \tfrac{1}{2}[|100\rangle|\Phi_-\rangle + |010\rangle|\Psi_-\rangle + |100\rangle|\Phi_+\rangle + |111\rangle|\Psi_+\rangle], \tag{5}$$

with a maximum entanglement of $25 \ln 2$. It is apparent that the previous state does not contain correlations going beyond those for the bipartite case. Certainly, the concomitant MABK correlations amount to 2.1361, only 27% of the corresponding maximum possible value. For $N = 6$ qubits, we described in Ref. [7] a state with a maximum entanglement given by Eq. (3). This is a state for which all bipartitions are maximally mixed. The aforementioned state has the form

$$\begin{aligned}|\Phi_6\rangle = \tfrac{1}{4}\,[\,&|\Psi^+_{0,6}\rangle + |\Psi^+_{3,6}\rangle + |\Psi^+_{5,6}\rangle + |\Psi^+_{6,6}\rangle\\ &+|\Psi^+_{9,6}\rangle + |\Psi^+_{15,6}\rangle + |\Psi^+_{17,6}\rangle + |\Psi^+_{18,6}\rangle\\ &+|\Psi^+_{24,6}\rangle + |\Psi^+_{29,6}\rangle - (\,|\Psi^+_{10,6}\rangle + |\Psi^+_{12,6}\rangle\\ &+|\Psi^+_{20,6}\rangle + |\Psi^+_{23,6}\rangle + |\Psi^+_{27,6}\rangle + |\Psi^+_{30,6}\rangle)\,]. \qquad (6)\end{aligned}$$

B. Some preliminary results

When pursuing maximum entanglement for real states *only*, we encounter, for $N = 4$, the following state:

$$\begin{aligned}\left|\Phi^R_4\right\rangle = \frac{1}{2\sqrt{2}}\,&[|\Psi^-_{0,4}\rangle - |\Psi^+_{3,4}\rangle - |\Psi^+_{4,4}\rangle\\ &+\sqrt{2}|\Psi^+_{5,4}\rangle + \sqrt{2}|\Psi^-_{6,4}\rangle + |\Psi^-_{7,4}\rangle)]. \qquad (7)\end{aligned}$$

This state—which has null discord—is highly entangled, but does not reach the maximal value. Instead, it stays very close to it ($9.2017 \ln 2$). Specifically, for the state (7) all one-qubit reduced matrices are maximally mixed, as in the case of the state (2), and two of the six associated density matrices for two qubits are maximally mixed. In the light of these results, we should require some figure of merit to somehow validate one of these two states or both of them.

Our real state of four qubits has $\mathrm{MABK}^{\max}_4 = \sqrt{6}$, only 43% of the maximum value (compare with 38% above). In our case $|\Phi^R_4\rangle$ is more nonlocal than $|\Phi_4\rangle$, although less entangled. In this case, the state possessing maximum correlations, *is not the one with complex coefficients*. Therefore, it seems to make some difference which field of numbers we use for building up quantum states.

Remarkably enough, Tapiador *et al.* [8] were able to algebraically recast, for $N = 6$, state (6) into a form that greatly clarifies how correlations are distributed among subsystems. This state $|\Psi_6\rangle$ reads

$$\tfrac{1}{2}(|\Psi^+_{0,4}\rangle|\Psi^-\rangle + |\Psi^+_{3,4}\rangle|\Psi^+\rangle + |\Psi^+_{6,4}\rangle|\Phi^-\rangle + |\Psi^+_{5,4}\rangle|\Phi^+\rangle). \qquad (8)$$

It is plain from (8) that all correlations existing in this maximally entangled state are encoded via maximally correlated four-party and two-party subsystems. The maximal violation of the corresponding MABK Bell inequality for six qubits is only 2 (18% of the maximum value). In other words, state (8) may have maximum entanglement, but does not appreciably violate the corresponding MABK inequality. For this state all concomitant reduced density matrices of one, two, and three qubits are completely mixed. $|\Psi_6\rangle$ constitutes an example of a state which has found applications in quantum information processing [9,10].

C. More results: The cases of $N = 7$ and $N = 8$ qubits

We give these two particular instances special consideration. In the case of $N = 7$ qubits, since the state obtained in [7] is one with no easily discernible algebraic structure, one wonders whether a better form for that state might exist, for either real or complex state functions. A more detailed study is carried out here. A conjecture made in [7] establishes that there are no pure states of seven qubits with marginal density matrices for subsystems of one, two, or three qubits that are (all of them) *completely* mixed. In contrast to the case of the seven-qubit state reported in [7], we encounter other states that—although lacking a simple structure—all possess totally mixed one- and two-qubit marginal density matrices. Note that several highly entangled states of seven qubits were obtained in [8], without reaching an upper bound.

The aforementioned state of $N = 7$ qubits possesses a maximum entanglement of 105.7882. Certainly, its reduced states of two qubits are not (all) mixed, but in practice they can be considered as such. This is so because, for reduced states of two qubits, six of them possess entanglement $0.992\,05 \ln 2$, and the remaining 15, $0.997\,60 \ln 2$. This "imperfect" mixture surely is immaterial for practical purposes. As far as three-qubit marginal density matrices are concerned, 15 contain an entanglement of $0.979\,13 \ln 8$, and the remaining 20, $0.995\,41 \ln 8$. Although some more compact algebraic form for the seven-qubit maximally entangled state could in principle be found, that is not actually the case. Such a putative state should necessarily be complex, not real, to attain maximum entanglement, which is of paramount importance for our present discussion. In the light of these (our third here) results, we may ask the following questions:

(a) Does it make *physical* sense to have states that are not completely mixed?

(b) Should one expect a maximally entangled state to be endowed with some sort of hierarchy in which increasing entanglement would be accompanied by maximal mixedness at every one-, two-, and three-qubit stages involving marginal states?

(c) Is it mandatory to resort to states with complex coefficients in order to have maximum multipartite entanglement?

Our main goal here is precisely to answer these questions in the present work. To this end we have explored the whole space of real and complex states via a simulated annealing method and have found similar results for both real and complex states. We have been able to detect states with totally mixed one- and two-qubit marginal density matrices, while increasing the mixedness for three qubits. In the case of $N = 7$ real states, we encountered a maximum entanglement of 105.1151, greater than that previously recorded. On the other hand, the instance of complex expansion coefficients displays a slightly greater value of entanglement than the real one, namely, 105.1441. While the former situation accrues nearly 31/35 completely mixed three-qubit reduced density matrices, in the latter that figure is increased up to 33/35. In Fig. 1, the coefficients of the real state are depicted. Had we let the optimization procedure evolve freely *in the complex case*, we would have reached the same result as in [7]. In other words, it is possible to obtain highly entangled states, either real or complex, with totally mixed one- and two-qubit reduced states.

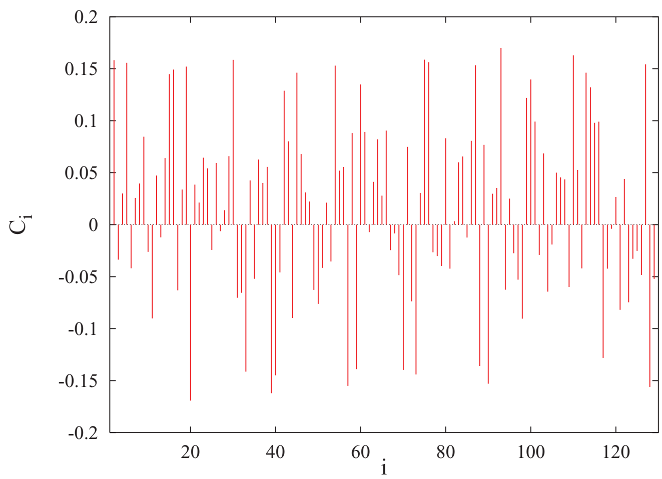

FIG. 1. (Color online) Coefficients of the real state of $N = 7$ qubits that maximizes total entanglement, with fully one- and two-qubit reduced states that are maximally mixed. See text for details.

On the whole, although we have not been able to provide a conclusive answer regarding entanglement for the $N = 7$ qubit case, we have shed light on the characteristics of these states by introducing one that possesses maximally mixed reduced two-qubit states. As we have seen, real and complex states behave differently, a situation that might become immaterial, provided real states suffice to fulfill eventual applications. All $N = 7$ qubit instances do not violate the corresponding MABK inequality.

Now, the last case of interest, which has been quite elusive, is the one corresponding to $N = 8$ qubits. It is undeniable that as we increase the dimension of the concomitant Hilbert space more and more, the problem of obtaining an optimum state with maximum generalized entanglement becomes less and less tractable, either analytically or numerically.

In any case, we have carried out extensive computations in order to get a suitable result. By performing a simulated annealing optimization procedure, we have reached a maximum for the entanglement and, in turn, obtained a multipartite state of eight qubits that appears to be an optimal one. We mention that in order to tackle the problem, we have pursued only real states, that is, configurations of states with real coefficients. This fact may limit the validity of our conclusions, but we are confident that, in any case, we have obtained a valid result. In addition, we have limited the expansion coefficients to be all equal in modulus, thus acquiring a *simple* algebraic structure. Needless to say, these simplifications have led to greater values of entanglement than arbitrary explorations with no constraints.

Our special state of eight qubits $|\Phi_8\rangle$ reads

$$\begin{aligned}\frac{1}{4\sqrt{2}}[&-|\Psi^-_{0,8}\rangle - |\Psi^-_{3,8}\rangle + |\Psi^-_{5,8}\rangle - |\Psi^-_{6,8}\rangle - |\Psi^+_{25,8}\rangle\\ &+|\Psi^+_{26,8}\rangle + |\Psi^+_{28,8}\rangle + |\Psi^+_{31,8}\rangle + |\Psi^-_{33,8}\rangle - |\Psi^-_{34,8}\rangle\\ &+|\Psi^-_{36,8}\rangle + |\Psi^-_{39,8}\rangle + |\Psi^+_{56,8}\rangle + |\Psi^+_{59,8}\rangle + |\Psi^+_{61,8}\rangle\\ &-|\Psi^+_{62,8}\rangle + |\Psi^-_{73,8}\rangle + |\Psi^-_{74,8}\rangle + |\Psi^-_{76,8}\rangle - |\Psi^-_{79,8}\rangle\\ &+|\Psi^+_{80,8}\rangle - |\Psi^+_{83,8}\rangle + |\Psi^+_{85,8}\rangle + |\Psi^+_{86,8}\rangle - |\Psi^-_{104,8}\rangle\\ &+|\Psi^-_{107,8}\rangle + |\Psi^-_{109,8}\rangle + |\Psi^-_{110,8}\rangle - |\Psi^+_{113,8}\rangle\\ &-|\Psi^+_{114,8}\rangle + |\Psi^+_{116,8}\rangle - |\Psi^+_{119,8}\rangle)].\end{aligned} \tag{9}$$

It exhibits interesting features. The amount of total entanglement is $362 \ln 2$. All reduced states of one, two, and three qubits are maximally mixed. This fact implies that this state is perfectly suitable for (i) performing teleportation protocols involving up to three qubits within eight parties, as well as (ii) many other applications. However, as expected, all four-qubit reduced states are not completely mixed. The work by Gisin and Bechmann-Pasquinucci [11] already pointed out that states of eight qubits cannot have all subsystems completely mixed. However, in our case, we get close enough to this desideratum.

Out of the $\binom{8}{4} = 70$ possible reduced states of four qubits:

(a) 56 matrices are completely mixed ($\ln 16$).

(b) Six of them are nearly diagonal matrices with four equal eigenvalues ($\frac{1}{2}\ln 16$). The corresponding partitions are {1,2,3,6},{1,2,4,5},{1,2,7,8},{3,4,5,6}, {3,6,7,8},{4,5,7,8}.

(c) The eight remaining matrices are almost diagonal, possessing eight equal eigenvalues ($\frac{3}{4}\ln 16$). The concomitant partitions are {1,3,4,7},{1,3,5,8},{1,4,6,8},{1,5,6,7}, {2,3,4,8},{2,3,5,7},{2,4,6,7},{2,5,6,8}.

State (9) does not violate the corresponding MABK Bell inequality. In the light of the previous results, we may formulate the following conjecture.

Conjecture 1. No maximally entangled state greater than five qubits violates the MABK Bell inequalities.

Summarizing the results of this section: (1) we confirm that no states of $N = 8$ qubits exist with all their marginal density matrices being maximally mixed and (2) we provided an example of a real state that might be tailored for quantum communication protocols or teleportation.

III. MAXIMALLY ENTANGLED STATES OF HIGHER DIMENSIONS

A. Preliminaries

Maximum qudit entanglement constitutes an extension of a previous study for qubits to states existing in a D^N Hilbert space, where D stands for the dimension of each party. Helwig *et al.* [12] addressed the interesting and nontrivial problem of finding the conditions for the existence of states that maximize the entanglement between all bipartitions. These states are of the type $|\Psi_{N,D}\rangle = \sum_{i=0}^{D^N-1} c_i|i\rangle$. The equivalence between several pure-state quantum secret-sharing schemes and states with maximum multipartite (N,D) entanglement with an even number of parties is proven in [12], an equivalence which indirectly implies the existence of these maximally entangled states for an arbitrary number of parties, based on known results about the existence of quantum secret-sharing schemes.

B. Our results

We will try to ascertain just what sort of states can host a maximum amount of entanglement between their parties. Since no general procedure has yet been provided for studying what conditions these maximally entangled qudit states should fulfill, we shall resort to numerical explorations that will hopefully shed some insight into qudit systems that might not apply for qubits. As dimensional examples we have considered the cases $\mathcal{H}_3^{\otimes 3}$, $\mathcal{H}_4^{\otimes 3}$, $\mathcal{H}_3^{\otimes 4}$, and $\mathcal{H}_3^{\otimes 5}$.

1. Three qutrits

The case of three qutrits ($\mathcal{H}_3^{\otimes 3}$) is really exceptional, as we shall see. The Hilbert space $\mathcal{H}_3$ is spanned by the basis $\{|0\rangle,|1\rangle,|2\rangle\}$. The state $|\Psi_{N=3,D=3}\rangle$,

$$\frac{1}{\sqrt{6}}[\,|000\rangle - |011\rangle - |112\rangle + |120\rangle - |202\rangle + |221\rangle\,], \quad (10)$$

possesses maximum entanglement 3 ln 3 and, from inspection, it is biseparable. The situation becomes more involved when one notices that the state

$$|\Psi'_{N=3,D=3}\rangle = \frac{1}{\sqrt{3}}[\,|000\rangle + |111\rangle + |222\rangle], \qquad (11)$$

which is clearly nonlocal, also reaches the maximum value 3 ln 3. How is it possible that two different states (one being separable, and the other nonseparable) may attain the same entanglement-based correlations? Should we use (11) and regard state (10) as an anomaly, or should we reconsider instead the definition of maximum entanglement?

Increasing individual party dimensions by one unit, we get a state existing in the Hilbert space $\mathcal{H}_4^{\otimes 3}$ (spanned by $\{|0\rangle,|1\rangle,|2\rangle,|3\rangle\}$). The maximally entangled state for $N = 3, D = 4$, $|\Psi_{3,4}\rangle$, reads

$$\frac{1}{2\sqrt{2}}[\sqrt{2}|002\rangle + \sqrt{2}|310\rangle - |121\rangle + |123\rangle + |231\rangle + |233\rangle]. \qquad (12)$$

This dimension does not pose the puzzle we found previously for three qutrits, in the sense that it is maximally entangled (3 ln 4) as opposed to

$$|\Psi'_{3,4}\rangle = \tfrac{1}{2}[\,|000\rangle + |111\rangle + |222\rangle + |333\rangle\,], \qquad (13)$$

which has entanglement $\frac{5}{4}\ln 4$. For (12), the first two elements are inseparable, while the remaining ones are biseparable. Thus, the role of quantum correlations is not as dominant as above. To be more rigorous, we should develop some tight Bell inequality and resort to the concomitant maximum violation. Unfortunately, no such Bell inequalities have been encountered so far.

2. Four qutrits

The case of four qutrits ($\mathcal{H}_3^{\otimes 4}$) is the natural extension of the four-qubit state. The state we obtain is of the form

$$\begin{aligned}|\Psi_{N=4,D=3}\rangle = \tfrac{1}{6}(&|0000\rangle + |1000\rangle + |0021\rangle + |1021\rangle\\ &+|0100\rangle - |0110\rangle - |0121\rangle - |0122\rangle\\ &+|0201\rangle - |0202\rangle + |0211\rangle + |0220\rangle\\ &-|1100\rangle - |1110\rangle + |1121\rangle - |1122\rangle\\ &-|1201\rangle - |1202\rangle + |1211\rangle - |1220\rangle)\\ &+\frac{\sqrt{2}}{6}(-|0012\rangle + |1012\rangle - |2001\rangle + |2020\rangle\\ &-|2102\rangle - |2111\rangle - |2210\rangle + |2222\rangle). \end{aligned} \qquad (14)$$

A careful analysis shows that the above state can be written as a combination of tensor products, where only bipartite correlations appear. These loose correlations in the four-party case should be contrasted with the corresponding ones for four-qubit states, where maximum entanglement is reached for (i) a state with complex expansion coefficients (linear combination of three maximally correlated states) and (ii) real ones (states with high but not maximum entanglement embedded into a linear combination of six maximally correlated states). The differences between the cases of maximum entanglement between $(N, D = 2)$ and arbitrary (N, D) have to be taken into account in order to shed light on the problem of quantifying and characterizing entanglement for multipartite systems.

3. Five qutrits

The case of five qutrits ($\mathcal{H}_3^{\otimes 5}$) has turned out to be elusive. We cannot provide a simple expression for the concomitant state, only an approximate one. However, numerical evidence shows, in a "real" quantum treatment, it is most likely that a maximum entanglement (25 ln 3) might be reached, that is, all reduced states of one and two qubits are likely to be maximally mixed. However, this is just an approximate result. If it were confirmed, this would entail that, in greater dimensions, real expansion coefficients suffice to describe all sorts of states with maximum correlations. This fact has been confirmed for the case $(N = 3, D = 5)$ $(S = 3\ln 5)$ as well, but the concomitant state can not be cast in simple fashion. In view of the previous results, we formulate a second conjecture.

Conjecture 2. Maximally entangled states of multiqudit systems (N, D) require only real expansion coefficients. Also, all their reduced density matrices are completely mixed.

For multiqubit states, in only a few cases are all reduced density matrices proportional to the normalized identity (that is, maximum entanglement), whereas in the case of qudits the instances encountered do not display this behavior. Furthermore, it is important to use complex expansion coefficients for qubits to get maximum entanglement, but this constraint disappears in higher dimensions. These are issues of great interest that find at least partial elucidation in the present work.

IV. MULTIQUBIT STATES WITH MAXIMAL DISCORD

A. Preliminaries: Geometric discord

The geometric measure of quantum discord (GQD) is a measure introduced so as to grasp all properties of the usual discord measure. Remember that the geometric measure of quantum discord, with χ a generic state with zero quantum discord, is given by the Hilbert-Schmidt norm

$$\mathrm{GQD}(\rho) = \mathrm{Min}_\chi[||\rho - \chi||^2], \qquad (15)$$

where the minimum is taken over the set of zero-discord states χ. This is of the form [13]

$$\begin{aligned}\mathrm{GQD}(\rho) &= \frac{1}{4}(||\mathbf{x}||^2 + ||T||^2 - \lambda_{\max})\\ &= \frac{1}{R} - \frac{1}{4} - \frac{1}{4}(||\mathbf{y}||^2 + \lambda_{\max}),\end{aligned} \qquad (16)$$

where $||\mathbf{x}||^2 = \sum_u x_u^2$, $\lambda_{\max}$ is the maximum eigenvalue of the matrix $(x_1,x_2,x_3)^t(x_1,x_2,x_3) + TT^t$, and $R = 1/\mathrm{Tr}(\rho^2)$.

In the case of entanglement, the most straightforward way of tackling quantum correlations in multipartite states is to introduce partitions into the system. This seems inevitable, as

TABLE I. Expansion coefficients for the states of three qubits that maximize the total GQD between pairs. The columns refer to real and complex coefficients. See text for details.

Coefficient	Real state	Complex state
c_0	0.435569236	(0.0546370323,−0.100659299)
c_1	−0.186434446	(0.0134949587,−0.188315179)
c_2	0.151369915	(0.465863387,0.0484337848)
c_3	−0.0680793253	(0.242430776,−0.0818648344)
c_4	−0.177771681	(0.136790716,−0.217618993)
c_5	−0.676301307	(−0.500174131,0.0275624382)
c_6	−0.505730715	(−0.442832499,0.0730590501)
c_7	0.0567821074	(0.0598215336,−0.379958264)

no definitive entanglement measure or criterion is yet available for characterizing true multipartite quantum correlations of this kind. Since QD is defined only between pairs of qubits, it is quite natural to extend the same tools used for multipartite entanglement to the case of quantum discord. If not otherwise stated, all states are given in the computational basis $\{|000\ldots00\rangle, |000\ldots01\rangle, |000\ldots10\rangle, \ldots, |111\ldots10\rangle, |111\ldots11\rangle\}$. This is a computable quantity that detects (and quantifies) true discord.

B. Our results

1. $N = 3$

The case of $N = 3$ qubits is special, because the result we obtain is a rather simple one, although the associated state is, instead, of a rather involved nature. When approaching the problem of finding a state $\rho = |\phi\rangle\langle\phi|$ of three qubits where $\mathrm{GQD}(\rho_{12}) + \mathrm{GQD}(\rho_{13}) + \mathrm{GQD}(\rho_{23})$ is maximum, by definition.

One assumes that the outcome for the unknown expansion coefficients is not going to be a simple one. Indeed, by the nature of this measure, we obtain via simulated annealing what appear to be random coefficients for the state $\rho = |\phi\rangle\langle\phi|$. This fact should not surprise anyone since the mathematical restrictions that are imposed when optimizing the sum of the GQD content for all pairs are highly nonlinear. Table I lists the real and complex coefficients –in the computational basis, which yield the same maximum GQD.

The concomitant maximum GQD is equal to 5/8, but *individual* discords are different. That is, $\mathrm{GQD}(\rho_{12}) = 1/8$, $\mathrm{GQD}(\rho_{13}) = 1/4$, and $\mathrm{GQD}(\rho_{23}) = 1/4$. Apparently, there is no *a priori* reason for this to be the case. This asymmetry between pairs constitutes the first discord feature that is different from those pertaining to the generalized entanglement measure in multipartite systems. Strictly speaking, states with maximal entanglement do have reduced states with different entanglement values, but this occurs only for large number of reduced-state qubit bipartitions. This sort of "GQD-asymmetry" occurs already in the simplest possible case of $N = 3$ qubits and poses a conundrum.

Although there is an alternative measure for computing the discord content of a given state, we prefer the usual quantum discord definition

$$\mathrm{QD} = \sum_i \mathrm{QD}[\rho_i], \tag{17}$$

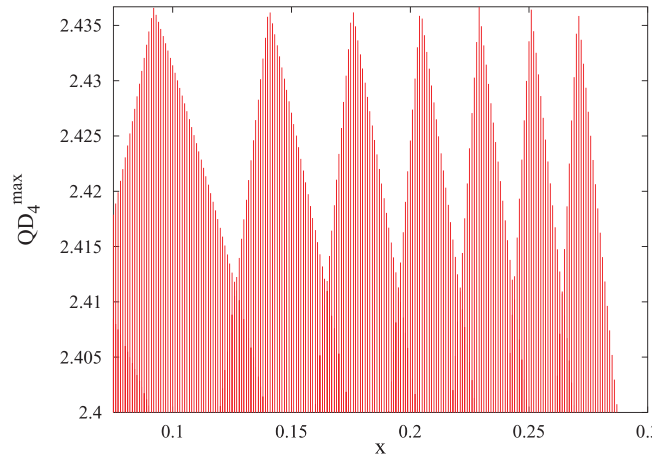

FIG. 2. (Color online) QD for the family of states (19) of $N = 4$ qubits. Seven x values clearly reach the maximum value. The $x = 0$ case is given by (20). See text for details.

where the sum takes place only over all $N(N-1)/2$ reduced two-qubit states ρ_i, since QD is defined only in that case. We stress here that the computation of the maximum QD is a twofold optimization procedure: first, one must find, given an arbitrary state, the minimum QDs for all pairs ρ_{ij}, and then survey all states until the maximum QD is attained.

It would appear that since $N = 3$ qubits is a low-dimensional system, the state maximizing the concomitant QD should be given by an algebraically simple expression. As in the case of the previous GQD measure, this is not the case. The $N = 3$ qubits case leads the result $QD = 1.662\,026$, given by the state

$$\begin{aligned} \left|\Psi_3^{\mathrm{QD}}\right\rangle = {} & 0.528\,95|000\rangle + 0.194\,92|001\rangle + 0.251\,44|010\rangle \\ & -0.482\,24|011\rangle + 0.382\,50|100\rangle - 0.398\,01|101\rangle \\ & -0.202\,13|110\rangle + 0.202\,09|111\rangle. \end{aligned} \tag{18}$$

The same asymmetry already found in the QGD case occurs here also. Also, real and complex states provide the same result. Here $\mathrm{MABK}_3^{\max} = 3.0430{,}76\%$ of the maximum possible violation, with an entanglement $2.7394 \ln 2$ (91%, very close to maximal). Thus, a state with maximum QD has a relatively high value for the several quantum correlations surveyed in this work.

2. $N = 4$

The $N = 4$ case leads to the result $\mathrm{QD} = 2.436\,681$, with partitions $\{1,2\},\{3,4\}$ having $\mathrm{QD} = 1/3$, and $\mathrm{QD} = 0.442\,503$ for the remaining pairs. This symmetry also occurs in the case of the computation of the GQD, equal to 1.045 667. We find the state $|\Psi_4^{\mathrm{QD}}\rangle$ to be of the type

$$\begin{aligned} & x\left(|\Psi_{2,4}^{-}\rangle + \tfrac{1}{2}|\Psi_{4,4}^{-}\rangle - \tfrac{1}{2}|\Psi_{7,4}^{-}\rangle\right) + z|\Psi_{3,4}^{+}\rangle + y|\Psi_{5,4}^{+}\rangle \\ & \quad + y|\Psi_{6,4}^{+}\rangle. \end{aligned} \tag{19}$$

For this family of states, the QD is plotted in Fig. 2 as a function of x. In addition to $x = 0$, there exist seven other states that reach the maximum possible QD value. The one we

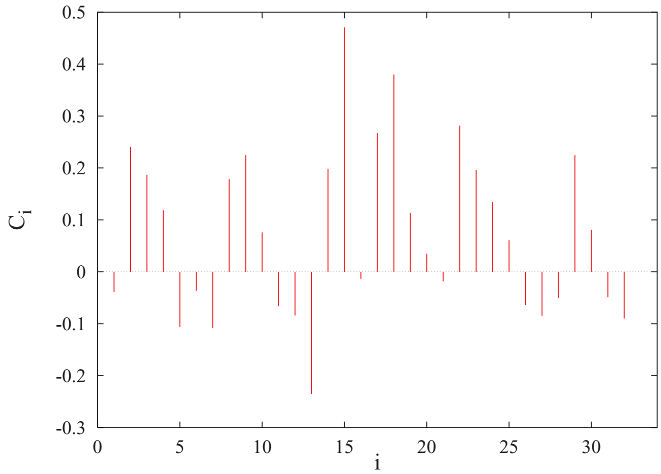

FIG. 3. (Color online) Coefficients of the state of $N = 5$ qubits maximizing QD. No clear algebraic structure can be drawn from these results. See text for details.

consider here is given in (19) with $x = 0$, that is,

$$|\Psi_4^{QD}\rangle = \frac{1}{\sqrt{3}}|\Psi_{3,4}^+\rangle + \frac{1}{2\sqrt{3}}|\Psi_{5,4}^+\rangle + \frac{1}{2\sqrt{3}}|\Psi_{6,4}^+\rangle. \quad (20)$$

Notice that this state has all its two-qubit reduced states of the X form. Accordingly, their QD is given in analytical fashion [14]. Note that the state that we have found to attain maximal QD does have the same maximally correlated substates as the maximally entangled state of four qubits (2). Needless to say, real and complex states reach the same maximum QD value. Finally, MABK$(|\Psi_4^{QD}\rangle) = \frac{8}{3}\sqrt{2}$ (67%).

3. $N = 5$

In the case of $N = 5$ qubits, we have not reached a "nice" algebraic form for the maximal state. All contributions in the computational basis possess a nonzero weight, and the overall state does not seem to exhibit any symmetry. However, within the limits of numerical accuracy, all $5(5-1)/2 = 10$ pairs of qubits seem to have the same amount of QD, the total being 3.642 445. This fact implies that there ought to be a simpler form for the aforementioned state. The expansion coefficients are shown in Fig. 3. The MABK correlations of the state $|\Psi_5^{QD}\rangle$ amount to ≈5.0233 (63%).

4. $N = 6$

The case of $N = 6$ qubits, on the other hand, does exhibit a definite symmetry. All reduced pairs have the same QD value (0.350 977) and the total QD is 5.264 662. As in the case of $N = 4$ qubits, all pairs are of the X form and, thus, analytically computable. The final (real) state is of the form

$$\begin{aligned}|\Psi_6^{QD}\rangle = \frac{1}{4\sqrt{5}}[&|\Psi_{0,6}^+\rangle + |\Psi_{3,6}^+\rangle + |\Psi_{5,6}^+\rangle + |\Psi_{6,6}^+\rangle \\ &+ |\Psi_{9,6}^+\rangle + |\Psi_{10,6}^+\rangle + |\Psi_{12,6}^+\rangle + |\Psi_{15,6}^+\rangle \\ &+ |\Psi_{17,6}^+\rangle + |\Psi_{18,6}^+\rangle + |\Psi_{20,6}^+\rangle + |\Psi_{23,6}^+\rangle \\ &+ |\Psi_{24,6}^+\rangle + |\Psi_{27,6}^+\rangle + |\Psi_{30,6}^+\rangle + 5|\Psi_{29,6}^+\rangle]. \quad (21)\end{aligned}$$

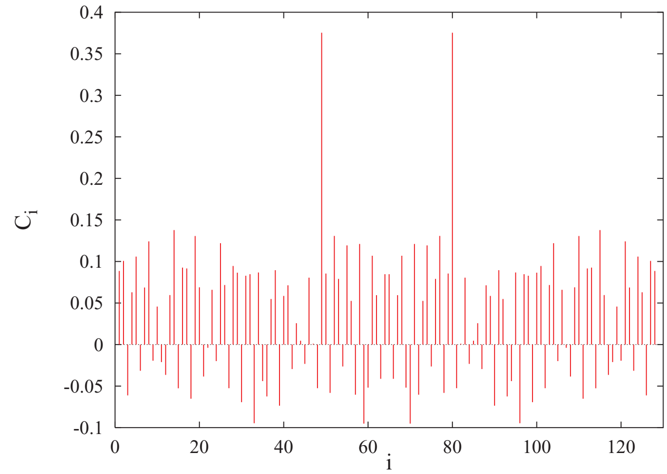

FIG. 4. (Color online) As for Fig. 3 for $N = 7$ qubits. A single state ($|\Psi_{48,7}^+\rangle$) significantly contributes to the total QD. Notice the symmetry between the i and $2^N - i$ coefficients, which constitutes a clear sign of an underlying superposition of maximally correlated states. See text for details.

Notice again the tendency towards a large number of linear combinations of maximally correlated states. Specifically, the state $|\Psi_{29,6}^+\rangle$ is particularly relevant. Again, complex and real coefficients lead to the same QD value.

5. $N = 7$

The case of $N = 7$ qubits is tantalizing. As in the case of $N = 5$ qubits, we have not been able to find a simple algebraic form. In contrast, our hypothesis of—as far as QD is concerned—a total symmetry in the state basis is duly confirmed here. That is, the state of seven qubits is formed by a plethora ($2^7/2 = 64$) of maximally correlated states. The state we obtain possesses a maximum QD of 8.4290, which is only an approximate value. Figure 4 shows the value of the expansion coefficient for each position in the computational basis. The two peaks correspond to the state $|\Psi_{48,7}^+\rangle$, which for unknown reasons becomes differentiated from the rest. Once again, complex and real coefficients are equivalent when providing states with maximum QD.

V. COMPARISON BETWEEN DIFFERENT MEASURES

At first sight, there is no precise way to correlate the measures S,MABK$_N^{max}$, and QD. However, although different in nature, they globally behave in analogous fashion. We observe that, in all three cases, the states' maximal measures for each quantum correlation type either increase or diminish exponentially with the number of parties. This behavior becomes apparent in Fig. 5. Now, when relating two definite measures, special instances appear. Let us consider the case of $N = 4$ qubits. It was shown that two states reached maximum "real" and "complex" entanglement separately. Additionally, the state maximizing entanglement is the only one of all the multiqubit states here considered that has nonzero QD. In general, entanglement and quantum discord are more similar to each other than to the state of affairs responsible for MABK violation.

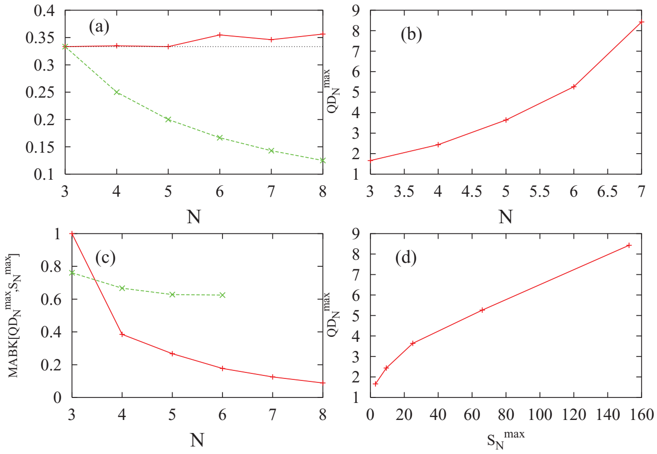

FIG. 5. (Color online) (a) Value of $S_N^{\max}$ vs N in terms of $[N(2^{N-1}-1)\frac{1}{3}\ln 2]$ (upper curve). $N=3$, and $N=5$ coincide (1/3, horizontal line). The remaining values display a steplike evolution. S_N for $|\mathrm{GHZ}_N\rangle$ states (maximally nonlocal) in units of the same quantity $[N(2^{N-1}-1)\frac{1}{3}\ln 2]$ is also depicted (lower curve). (b) Value of $\mathrm{QD}_N^{\max}$ vs N. The evolution is clearly exponential. (c) Normalized MABK correlations (to $2^{(N+1)/2}$) for maximally entangled (solid line) and discordant (dot-dashed line) qubit states. The QD case saturates to $k2^{(N+1)/2}$, k being some positive constant, for an increasing number of parties. (d) $\mathrm{QD}_N^{\max}$ vs $S_N^{\max}$. Notice that each point corresponds to different states. On the whole, a monotonically increasing behavior is apparent. See text for details.

Regarding MABK correlations vs entanglement, it is plain from Table II that maximum entanglement by no means implies maximum MABK correlation. Nevertheless, $\mathrm{MABK}_N^{\max}$ is not very different from maximum entanglement. This fact is easily seen when analyzing generalized GHZ states, which are the ones that maximize MABK Bell inequalities. The measure $\mathrm{MABK}_N^{\max}$ is equal to $2^{(N+1)/2}$, and its entanglement is $S_N(|\mathrm{GHZ}_N\rangle) = (2^{N-1}-1)\ln 2$ $[\mathrm{QD}_N(|\mathrm{GHZ}_N\rangle)=0]$. The entanglement and $\mathrm{MABK}_N^{\max}$ for generalized GHZ states are

TABLE II. Several types of correlation measure for states with increasing number of qubits. The first column displays the maximum violation of the generalized MABK Bell inequality for those states that maximize the generalized measure of entanglement, as well as the concomitant percentage with respect to the maximum possible violation ($2^{(N+1)/2}$ for each N). The second column displays similar results for those states with maximum QD. Finally, in the last column, the entanglement for states maximizing QD is computed. Notice that some results are analytic. The computation of QD for states with maximum entanglement is not depicted, as it vanishes except for $N=4$ $[\mathrm{QD}(S_{\max})=0.7548\ (31\%)]$. See text for details.

N	$\mathrm{MABK}(S_{\max})$	$\mathrm{MABK}(\mathrm{QD}_{\max})$	$S(\mathrm{QD}_{\max})$
3	4 (100%)	3.0430 (76%)	$2.7394\ln 2$ (1%)
4	2.1773 (38%)	$\frac{8}{3}\sqrt{2}$ (67%)	$8\ln 2$ (5%)
5	2.1381 (27%)	≈5.0233 (63%)	$17.7864\ln 2$ (1%)
6	2 (18%)	$5\sqrt{2}$ (62.5%)	$41.2542\ln 2$ (3%)
7	2 (13%)	≈7.2524 (45%)	≈$97.9457\ln 2$ (4%)
8	2 (9%)		

monotonically increasing functions one of the other

$$\to S_N = \left(\tfrac{1}{4}\left[\mathrm{MABK}_N^{\max}\right]^2 - 1\right)\ln 2. \tag{22}$$

The average entanglement per partition is equal to $\ln 2$ in all cases. When computing the maximum entanglement for qubit systems, we obtain that

$$S_N^{\max} \geqslant N(2^{N-1}-1)\tfrac{1}{3}\ln 2, \tag{23}$$

equality holding for $N=3,5$. In Fig. 5(a) we depict $S_N^{\max}$ and $S_N(|\mathrm{GHZ}_N\rangle)$ in terms of $[N(2^{N-1}-1)\frac{1}{3}\ln 2]$ vs N. What we obtain is that the entanglement for maximally entangled states behaves in the same way, differences appearing between clusters of states (states of three, four, and five qubits are to be compared with results for six, seven, and eight qubits). A kind of steplike behavior is apparent, as well as the decreasing tendency of $S_N(|\mathrm{GHZ}_N\rangle)$. This fact shows that MABK correlations display a special behavior, as opposed to the relation of entanglement vs discord, where general tendencies are more pronounced.

$\mathrm{QD}_N^{\max}$ for each number of qubits is depicted in Fig. 5(b). This curve is perfectly fitted by an exponential. Thus, maximum QD also evolves exponentially with the number of parties involved. As far as MABK violation is concerned, Fig. 5(c) displays the evolution of MABK correlations for those states with maximal discord (dot-dashed line) and maximum entanglement (solid line) in units of $2^{(N+1)/2}$. It is plain that MABK violation for maximally entangled states diminishes exponentially, whereas in the case of quantum discord, a sort of proportionality is reached $[\mathrm{MABK}(\mathrm{QD}_N^{\max}) \propto 2^{(N+1)/2}$ for $N \geqslant 7]$.

When comparing maximum quantities corresponding to different states, we obtain a result such as the one depicted in Fig. 5(d). That is, the QDs for those states maximizing QD monotonically increases with their entanglement counterparts.

VI. CONCLUSIONS

Some interesting discoveries derive from our exploration of the tripod entanglement-discord-MABK correlations in the case of multiqubit systems.

(1) We first reconsidered the known cases of maximally entangled states of $N=4$, 5, and 6 qubits, with the intent of ascertaining here their properties as far as MABK violation is concerned. The cases of 7 and 8 qubits have been studied with somewhat more detail.

(2) It has become clear that, some similarities notwithstanding, entanglement and $\mathrm{MABK}_N^{\max}$ correlations behave differently. Recall, however, that we focus only on extreme cases, and not on arbitrary states. The aforementioned tendency has been confirmed for an increasing number of qubits.

(3) Quantum discord has been extended here to multiqubit systems by introducing a measure over all two-qubit partitions. Employing the corresponding maximum value, we have discovered states of "maximum discord" for up to eight qubits. These states possess very interesting features, including unexplained asymmetries among their parties.

(4) We have also explored entanglement in multiqudit systems, and obtained the concomitant maximally entangled states for different (N,D) configurations. Also, the way of defining quantum mechanics over real or complex numbers

is subject to inspection here. We find that real expansion coefficients in a given basis suffice to explain maximum entanglement. Recall that this was not the case for multiqubit states.

(5) Finally, the comparison of all types of measure leads us to conclude that entanglement and discord are positively correlated, whereas MABK correlations decrease with either maximum entanglement or discord. We conclude, thus, that maximum entanglement and maximum discord display some similarities, whereas this scenario is blurred when considering MABK correlations.

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