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Multipartite entanglement and frustration

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Abstract. Some features of the global entanglement of a composed quantum system can be quantified in terms of the purity of a balanced bipartition, made up of half of its subsystems. For the given bipartition, purity can always be minimized by taking a suitable (pure) state. When many bipartitions are considered, the requirement that purity be minimal for all bipartitions can engender conflicts and frustration will arise. This unearths an interesting link between frustration and multipartite entanglement, defined as the average purity over all (balanced) bipartitions.

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Contents

1. Introduction

Frustration in humans and animals arises from unfulfilled needs. Freud related frustration to goal attainment and identified inhibiting conditions that hinder the realization of a given objective [1]. In the psychological literature one can find many diverse definitions but, roughly speaking, a situation is defined as frustrating when a physical, social, conceptual or environmental obstacle prevents the satisfaction of a desire [2]. Interestingly, definitions of frustration have appeared even in the jurisdictional literature and appear to be related to an increased incidence of parties seeking to be excused from performance of their contractual obligations [3]. There, 'Frustration occurs whenever the law recognises that without default of either party, a contractual obligation has become incapable of being performed because the circumstances in which performance is called for would render it a thing radically different from that which was undertaken by the contract.... It was not this I promised to do' [4].

In physics, this concept must be mathematized. A paradigmatic example [5] is that of three characters, A, B and C, who are not good friends and do not want to share a room. However, there are only *two* available rooms, so that at least two of them will have to stay together. Therefore their needs will not be fulfilled and frustration will arise. A schematic mathematical description of this phenomenon consists of assigning a 'coupling' constant J_{ik} to each couple (i, k), with $i, k = A, B, C$: $J_{ik} = +1(-1)$ if i and k (do not) like to share a room. Each character is then assigned a dichotomic variable $S_i = +1(-1)$ if i is in the first (second) room. The key ingredient is the definition of a *cost function* that quantifies the amount of 'discomfort' (unfulfilled needs) of our three characters. This can be easily done:

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ik} S_i S_k. \tag{1}$$

The goal is to minimize this cost. In our case $J_{ik} = -1$, $\forall i, k$, so that

$$H = S_A S_B + S_A S_C + S_B S_C. \tag{2}$$

Each addendum in the summation can take only two values, ± 1. However, although each single addendum can be made equal to -1 (separate rooms, minimum cost and no discomfort for the given couple), their sum, in the best case, is $H_{\min} = -1$, which is larger than the sum of the three minima, -3. At least two characters will have to share a room and frustration arises. This is a typical case of frustrated antiferromagnetic coupling on a (very small) triangular lattice. The situation becomes more complicated (and interesting) when more characters are involved and the coupling constants in (1) are, e.g., statistically distributed. A typical result is obtained when the couplings J_{ik}'s are randomly and independently distributed dichotomic variables (± 1). In such a case, given N characters, $H/N^{3/2} \simeq -0.7633$ for almost all realizations of the J_{ik}'s. In other words, there is minimum discomfort (cost) when each character shares a room with a number of enemies that is slightly smaller than if the room had been decided by tossing a coin [5]. Many other interesting situations can be conceived, according to the statistical distribution of the couplings and the number or characters and possibilities involved.

The above description of frustration, in terms of a cost function, applies to a classical physical system. Interestingly, there is a frustration associated with quantum entanglement in many-body systems. The study of this problem will be the aim of the present investigation.

Entanglement is a very characteristic trait of quantum mechanics that was identified at the inception of the theory [6]–[8], has no analogue in classical physics [9], and has come to be considered as a resource in quantum information science [10, 11]. When the system is bipartite, its entanglement can be unambiguously quantified in terms of the von Neumann entropy or the entanglement of formation [12, 13]. Difficulties arise, however, when one endeavors to define *multipartite* entanglement [14]–[18]. The main obstacle comes from the fact that states endowed with large entanglement typically involve exponentially many coefficients and cannot be quantified with a few measures. This interesting feature of multipartite entanglement, already alluded to in [19], motivated us to look for a statistical approach [20], based on the characterization of entanglement that makes use of the probability density function of the entanglement of a subsystem over all (balanced) bipartitions of the total system [21]. A state has a large multipartite entanglement if its average bipartite entanglement is large (and is possibly also largely independent of the bipartition).

Maximally multipartite entangled states (MMES) [22, 23] are states whose entanglement is maximal for every (balanced) bipartition. The study of MMES has brought to light the presence of frustration in the system, highlighting the complexity inherent in the phenomenon of multipartite entanglement. Frustration in MMES is due to a 'competition' among bipartitions and the impossibility of fulfilling the requirement of maximal entanglement for all of them, given the quantum state [20, 22]. The links between entanglement and frustration were also investigated in [24]–[27].

This paper is organized as follows. We introduce notation and define maximally bipartite entangled states and MMES in section 2. We numerically investigate these states and show that multipartite entanglement is a complex phenomenon and exhibits frustration, whose features are studied in section 3. Section 4 contains our conclusions and an outlook.

2. From bipartite to multipartite entanglement

The notion of MMES was originally introduced for qubits [22] and then extended to continuous variable systems [28, 29]. Here we follow [29] and give a system-independent formulation. Consider a system composed of n identical (but distinguishable) subsystems. Its Hilbert space $\mathcal{H} = \mathcal{H}_S$, with $\mathcal{H}_S := \bigotimes_{i\in S} \mathfrak{h}_i$ and $S = \{1, 2, \ldots, n\}$, is the tensor product of the Hilbert spaces of its elementary constituents $\mathfrak{h}_i \simeq \mathfrak{h}$. Examples range from qubits, where $\mathfrak{h} = \mathbb{C}^2$, to continuous variable systems, where $\mathfrak{h} = L^2(\mathbb{R})$. We will denote a bipartition of system S by the pair $(A, \bar{A})$, where $A \subset S$, $\bar{A} = S \setminus A$ and $1 \leqslant n_A \leqslant n_{\bar{A}}$ ($n_A + n_{\bar{A}} = n$), with $n_A = |A|$, the cardinality of party

A (i.e. the number of elements of A). At the level of Hilbert spaces, we obtain

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\bar{A}}. \tag{3}$$

Let the total system be in a (normalized) pure state $|\psi\rangle \in \mathcal{H}$, which is the only case we will consider henceforth. The amount of entanglement between party A and party $\bar{A}$ can be quantified, for instance, in terms of the purity

$$\pi_A = \mathrm{tr}(\rho_A^2) \tag{4}$$

of the reduced density matrix of party A,

$$\rho_A = \mathrm{tr}_{\mathcal{H}_{\bar{A}}}(|\psi\rangle\langle\psi|). \tag{5}$$

Purity ranges between

$$\pi_{\min}^{n_A} \leqslant \pi_A \leqslant 1, \tag{6}$$

where

$$\pi_{\min}^{n_A} = (\dim \mathcal{H}_A)^{-1} = (\dim \mathfrak{h})^{-n_A}, \tag{7}$$

with the stipulation that $1/\infty = 0$. The upper bound 1 is attained by unentangled, factorized states $|\psi\rangle = |\phi\rangle_A \otimes |\chi\rangle_{\bar{A}}$ (according to the given bipartition). When $\dim \mathfrak{h} < \infty$, the lower bound, that depends only on the number of elements n_A composing party A, is attained by maximally bipartite entangled states, whose reduced density matrix is a completely mixed state

$$\rho_A = \pi_{\min}^{n_A} \mathbf{1}_{\mathcal{H}_A}, \tag{8}$$

where $\pi_{\min}^{n_A}$ is defined in equation (7) and $\mathbf{1}_{\mathcal{H}_A}$ is the identity operator on $\mathcal{H}_A$. This property is valid at fixed bipartition $(A, \bar{A})$; we now try and extend it to more bipartitions.

Consider the average purity ('potential of multipartite entanglement') [22, 30]

$$\pi_{\mathrm{ME}}^{(n)}(|\psi\rangle) = \mathbb{E}[\pi_A] = \frac{1}{C_{n_A}^n} \sum_{|A|=n_A} \pi_A, \tag{9}$$

where $\mathbb{E}$ denotes the expectation value, $C_{n_A}^n$ is the binomial coefficient, $|A|$ is the cardinality of A and the sum is over balanced bipartitions $n_A = [n/2]$, $[\,\cdot\,]$ denoting the integer part. The quantity $\pi_{\mathrm{ME}}^{(n)}$ in equation (9) measures the average bipartite entanglement over all possible balanced bipartitions and inherits the bounds (6) (with $n_A = [n/2]$)

$$\pi_{\min}^{[n/2]} \leqslant \pi_{\mathrm{ME}}^{(n)}(|\psi\rangle) \leqslant 1. \tag{10}$$

A MMES [22] $|\varphi\rangle$ is a minimizer of π_{ME},

$$\pi_{\mathrm{ME}}^{(n)}(|\varphi\rangle) = E_0^{(n)}, \tag{11}$$
$$\text{with} \quad E_0^{(n)} = \min\{\pi_{\mathrm{ME}}^{(n)}(|\psi\rangle) \mid |\psi\rangle \in \mathcal{H}_S, \langle\psi|\psi\rangle = 1\}.$$

The meaning of this definition is clear: most measures of bipartite entanglement (for pure states) exploit the fact that when a pure quantum state is entangled, its constituents are in a mixed state. We are simply generalizing the above distinctive trait to the case of multipartite entanglement, by requiring that this feature be valid for all bipartitions. The density matrix of each subsystem $A \subset S$ of a MMES is as mixed as possible (given the constraint that the total system is in a pure state), so that the information contained in a MMES is as distributed as possible. The average purity introduced in equation (9) is related to the average linear entropy [30] and extends ideas put forward in [17, 31].

We shall say that a MMES is *perfect* when the lower bound (10) is saturated

$$E_0^{(n)} = \min\{\pi_{\mathrm{ME}}^{(n)}\} = \pi_{\min}^{[n/2]}. \tag{12}$$

It is clear that a necessary and sufficient condition for a state to be a MMES is that it be maximally entangled with respect to balanced bipartitions, i.e. those with $n_A = [n/2]$. Since this is a very strong requirement, perfect MMES may not exist for $n > 2$ (when $n = 2$ the above equation can be trivially satisfied) and the set of perfect MMES can be empty.

In the best of all possible worlds one can still seek for the (non-empty) class of states that better approximate perfect MMES, that is, states with minimal average purity. We shall say that a MMES is *uniformly optimal* when its distribution of entanglement is as fair as possible, namely when the standard deviation vanishes:

$$\sigma^{(n)} = \mathbb{E}\left[\left(\pi_A - \pi_{\mathrm{ME}}^{(n)}\right)^2\right]^{1/2} = 0, \tag{13}$$

where the expectation is taken according to the same distribution as in equation (9) (all balanced bipartitions). Of course, a perfect MMES is optimal. It is not obvious that uniformly optimal non-perfect MMES exist. We observe that states satisfying condition (13) exist, but are not necessarily MMES: think for instance of fully factorized states.

The very fact that perfect MMES may not exist is a symptom of frustration. We emphasize that this frustration is a consequence of the conflicting requirements that entanglement be maximal for all possible bipartitions of the system.

2.1. Qubits and symptoms of frustration

For qubits the total Hilbert space is $\mathcal{H}_S = (\mathbb{C}^2)^{\otimes n}$ and factorizes into $\mathcal{H}_S = \mathcal{H}_A \otimes \mathcal{H}_{\bar{A}}$, with $\mathcal{H}_A = (\mathbb{C}^2)^{\otimes n_A}$, of dimensions $N_A = 2^{n_A}$ and $N_{\bar{A}} = 2^{n_{\bar{A}}}$, respectively ($N_A N_{\bar{A}} = N$). Equations (6) and equations (10) and (11) read

$$1/N_A \leqslant \pi_A \leqslant 1, \tag{14}$$

$$1/N_A \leqslant E_0^{(n)} \leqslant \pi_{\mathrm{ME}}^{(n)}(|\psi\rangle) \leqslant 1, \qquad N_A = 2^{[n/2]}, \tag{15}$$

respectively.

For small values of n, one can tackle the minimization problem (11) both analytically and numerically. For $n = 2, 3, 5, 6$, the average purity saturates its minimum in (15): this means that purity is minimal *for all* balanced bipartitions. In this case the MMES is *perfect*.

For $n = 2$, (perfect) MMES are Bell states up to local unitary transformations, while for $n = 3$ they are equivalent to the GHZ states [32]. For $n = 4$ one numerically obtains $E_0^{(4)} = \min \pi_{\mathrm{ME}}^{(4)} = 1/3 > 1/4 = 1/N_A$ [22], [33]–[35]. For $n = 5$ and 6 one can find several examples of perfect MESS [22, 23]. The case $n = 7$ is still open, our best estimate being $E_0^{(7)} \simeq 0.13387 > 1/8 = 1/N_A$. Most interestingly, perfect MMES do not exist for $n \geqslant 8$ [30]. These findings are summarized in table 1 (left column) and bring to light the intriguing feature of multipartite entanglement we are interested in: since the minimum $1/N_A$ in equation (15) cannot be saturated, the value of π_A must be larger for some bipartitions A. We view this 'competition' among different bipartitions as a phenomenon of frustration: it is already present for n as small as 4. This frustration is the main reason for the difficulties one encounters in minimizing $\pi_{\mathrm{ME}}^{(n)}$ in (9). Note that the dimension of $\mathcal{H}_S$ is $N = 2^n$ and the number of partitions scales as N. We therefore need to define a viable strategy for the characterization of frustration in MMES, even for relatively small values of n.

Table 1. Comparison between qubit and Gaussian MMES for different values of number of subsystems, n.

n	Qubit perfect MMES	Gaussian perfect MMES
2,3	Yes	Yes
4	No	No
5,6	Yes	No, but uniformly optimal*
7	No*	No
$\geqslant 8$	No	No

*Numerical evidence.

2.2. Continuous variables and further symptoms of frustration

For continuous variables we have $\mathcal{H}_S = (L^2(\mathbb{R}))^{\otimes n}$ with $\dim L^2(\mathbb{R}) = \infty$. As a consequence, the lower bound $\pi_{\min}^{n_A} = 0$ in equation (7) is not attained by any state. Therefore, strictly speaking, in this situation there do not even exist maximally *bipartite* entangled states, but only states that approximate them. This inconvenience can be overcome by introducing physical constraints related to the limited resources one has in real life. This reduces the set of possible states and induces one to reformulate the question in the form: what are the physical minimizers of (4), namely the states that minimize (4) and belong to the set $\mathcal{C}$ of physically constrained states? In sensible situations, e.g. when one considers states with bounded energy and bounded number of particles, the purity lower bound

$$\pi_{\min}^{n_A,\mathcal{C}} = \inf\{\pi_A, |\psi\rangle \in \mathcal{C}\} \geqslant \pi_{\min}^{n_A} = 0 \tag{16}$$

is no longer zero and is attained by a class of minimizers, namely the *maximally bipartite entangled states*. If this is the case, we can also consider multipartite entanglement and ask whether there exist states in $\mathcal{C}$ that are maximally entangled for every bipartition $(A, \bar{A})$ and therefore satisfy the extremal property

$$\pi_A = \pi_{\min}^{n_A,\mathcal{C}} \tag{17}$$

for every subsystem $A \subset S$ with $n_A = |A| \leqslant n/2$. In analogy with the discrete variable situation, where $\dim \mathfrak{h} < \infty$ and $\mathcal{C} = \mathcal{H}$, we will call a state that satisfies (17) a *perfect MMES* (subordinate to the constraint $\mathcal{C}$).

Since, once again, the requirement (17) is very strong, the answer to this question can be negative for $n > 2$ (again, when $n = 2$ it is trivially satisfied) and the set of perfect MMES can be empty. In the best of the best of all possible worlds one can still seek the (non-empty) class of states that better approximate perfect MMES; that is, states with minimal average purity. In conclusion, by definition, a MMES is a state that belongs to $\mathcal{C}$ and minimizes the potential of multipartite entanglement (9). Obviously, when

$$E_0^{(n),\mathcal{C}} = \min_{\mathcal{C}}\{\pi_{\mathrm{ME}}^{(n)}\} = \pi_{\min}^{[n/2],\mathcal{C}} \tag{18}$$

there is no frustration and the MMES are perfect. Eventually, we will consider the limit $\mathcal{C} \to \mathcal{H}$.

Let us consider the quantum state $|\psi_{(n)}\rangle$ of n identical bosonic oscillators with (adimensional) canonical variables $\{q_k, p_k\}_{k=1,\ldots,n}$ and unit frequency (set $\hbar = 1$). An analogous description of the system can be given in terms of the Wigner function on the n-mode phase space

$$W_{(n)}(q,p) = \int \mathrm{d}^n y \langle q - y|\psi_{(n)}\rangle\langle\psi_{(n)}|q + y\rangle \mathrm{e}^{2\mathrm{i}\pi y\cdot p}, \tag{19}$$

where $q = (q_1, \ldots, q_n)$, $p = (p_1, \ldots, p_n)$, $y = (y_1, \ldots, y_n) \in \mathbb{R}^n$, and we have denoted by

$$|q \pm y\rangle = \otimes_{k=1}^{n} |q_k \pm y_k\rangle \tag{20}$$

the generalized position eigenstates. By definition, Gaussian states [36, 37] are those described by a Gaussian Wigner function. Introducing the phase-space coordinate vector $X = (X_1, \ldots, X_{2n}) = (q_1, p_1, \ldots, q_n, p_n)$, a Gaussian state has a Wigner function of the following form:

$$W_{(n)}(X) = \frac{1}{(2\pi)^n\sqrt{\det(\mathbb{V})}} \exp\left[-\frac{1}{2}(X - X_0)\mathbb{V}^{-1}(X - X_0)^{\mathrm{T}}\right], \tag{21}$$

where $X_0 = \langle X\rangle = \int X W_{(n)}(X)\, \mathrm{d}^{2n}X$ is the vector of first moments, and $\mathbb{V}$ is the $2n \times 2n$ covariance matrix, whose elements are

$$\mathbb{V}_{lm} = \langle (X_l - \langle X_l\rangle)(X_m - \langle X_m\rangle)\rangle. \tag{22}$$

For Gaussian states, purity is a function of the 'sub' determinant of the covariance matrix

$$\pi_A = \frac{1}{2^{n_A}\sqrt{\det(\mathbb{V}_A)}}, \tag{23}$$

$\mathbb{V}_A$ being the square submatrix defined by the indices pertaining to bipartition A. Clearly, $\pi_A \leqslant 1$.

The results of the search for perfect and uniformly optimal MMES with Gaussian states are summarized in the right-hand column of table 1 [29]. There are curious analogies and differences with qubit MMES. In particular, for $n \geqslant 8$, perfect MMES do not exist in both scenarios. Actually, for Gaussian states, frustration is present for $n \geqslant 4$; for the 'special' integers $n = 5, 6$, we notice that both for two-level and continuous variables systems the variance of the distribution of entanglement goes to zero; on the other hand, in the former case one can find perfect MMES, and in the latter case, MMES are uniformly optimal but not perfect.

3. Scrutinizing frustration

We now turn to detailed study of the structure of frustration. For the sake of concreteness, we shall first focus on qubits. Let us start from a few preliminary remarks. We observed that it is always possible to saturate the lower bound in (14)

$$\pi_A = 1/N_A \tag{24}$$

for a *given* balanced bipartition $(A, \bar{A})$ with $N_A = 2^{[n/2]}$. However, in order to saturate the lower bound in (15)

$$E_0^{(n)} = 1/N_A, \tag{25}$$

condition (24) must be valid for every bipartition in the average (9). As was mentioned in section 2.1, this requirement can be satisfied only for a very few 'special' values of n ($n = 2, 3, 5$ and 6; see table 1). For all other values of n this is impossible: different bipartitions 'compete' with each other, and the minimum $E_0^{(n)}$ of $\pi_{\mathrm{ME}}^{(n)}$ is strictly larger than $1/N_A$.

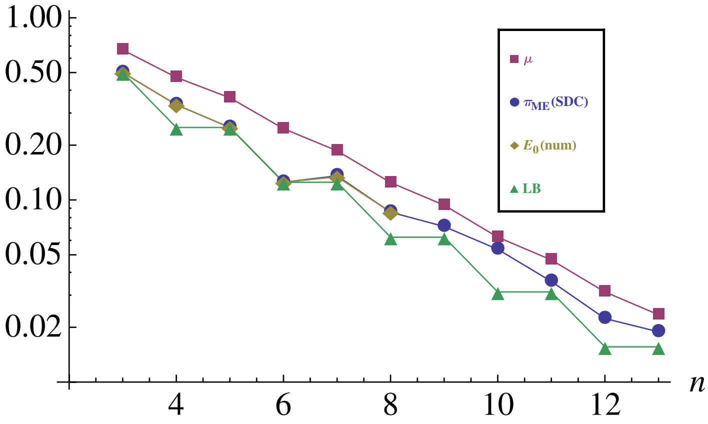

Figure 1. Qubits: average purity μ of the typical states (squares), average purity π_{ME}(SDC) computed according to Scott's procedure [30] with extremal additive self-dual codes (full circles), our best numerical estimate E_0(num) for the minimum of π_{ME} (diamonds) and lower bound LB $= 1/N_A$ (triangles) versus the number of spins n. Note that for $n = 7$ the full circle and diamond do not coincide. The scale on the ordinates is logarithmic.

It is interesting to look at this phenomenon in more detail. Let us recall that for typical states [21], [38]–[43], the distribution of purity over balanced bipartitions has mean

$$\mu^{(n)} = \frac{N_A + N_{\bar{A}}}{N+1}. \tag{26}$$

Figure 1 displays the average purity μ of typical states (equation (26)), the average purity of extremal additive self-dual codes states, computed according to Scott's procedure [30], our best numerical estimate for the minimum of $E_0^{(n)}$, and the lower bound $1/N_A$. All these quantities exponentially vanish as $n \to \infty$. Scott's states give an upper bound for the minimal average purity when $n \geqslant 8$, where the numerical simulations become very time consuming. In particular, we notice that for $3 \leqslant n \leqslant 6$ and $n = 8$ the numerical values of $E_0^{(n)}$ coincide with the results obtained using extremal additive self-dual codes [30]. For $n = 7$, the optimization algorithm reaches a lower value. For $n > 8$ our numerical data do not enable us to draw any conclusions.

Figure 2 displays the (normalized) difference between the minimum average purity, computed according to Scott's extremal additive self-dual codes and/or our best numerical estimate, and the lower bound $1/N_A$ in equation (25). This difference is an upper bound to the *frustration ratio*

$$F^{(n)} = \frac{E_0^{(n)} - 1/N_A}{E_0^{(n)}}, \qquad N_A = 2^{[n/2]} \tag{27}$$

that can be viewed as the 'amount of frustration' in the system. We notice the very different behaviors of $F^{(n)}$ for odd and even values of n. In the former case, the amount of frustration increases with the size of the system. On the contrary, in the latter case, the behavior is not monotonic. It would be of great interest to understand how this quantity behaves in the thermodynamical limit, but our data do not enable us to draw any clear-cut conclusions.

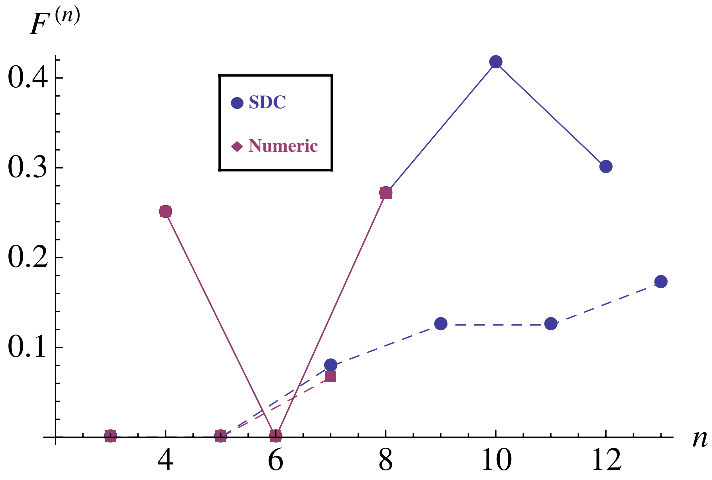

Figure 2. Qubits: frustration ratio: (normalized) distance between the average purity π_{ME}(SDC), according to Scott's extremal additive self-dual codes (full circles), or our best numerical estimate for the minimum E_0(num) (squares), and the lower bound LB $= 1/N_A$, versus the number of spins. Notice the difference between even and odd n.

Let us extend these considerations to the continuous variables scenario. In order to measure the amount of frustration (for states belonging to the constrained set $\mathcal{C}$), we define a more general frustration ratio

$$F^{(n),\mathcal{C}} = \frac{E_0^{(n),\mathcal{C}} - \pi_{\min}^{[n/2],\mathcal{C}}}{E_0^{(n),\mathcal{C}}} \tag{28}$$

and eventually take the limit $\mathcal{C} \to \mathcal{H}$, where both the numerator and the denominator can vanish. (Note that (27) is a specialization of the quantity in (28) to the qubit case, i.e. $\mathcal{C} = \mathcal{H} = (\mathbb{C}^2)^{\otimes n}$.) As a constraint we fix the value $\mathcal{N}$ of the average number of excitations per mode, namely

$$\mathcal{C} = \left\{ \psi \in \mathcal{H},\, \psi \text{ Gaussian},\, \frac{\langle q_k^2 + p_k^2 \rangle}{2} \leqslant \mathcal{N} + \frac{1}{2},\, 1 \leqslant k \leqslant n \right\}. \tag{29}$$

The ideal lower bound is given by [29]

$$\pi_{\min}^{[n/2],\mathcal{C}} = \frac{1}{2^{[n/2]}(\mathcal{N} + 1/2)^{[n/2]}} \tag{30}$$

and represents the purity of a Gaussian thermal state. Incidentally, we notice that, for $\mathcal{N} = 1/2$, equation (30) reproduces the lower bound of equation (15), i.e. the case of qubits. On the other hand, $\mathcal{N} = 0$ corresponds to the case of completely separable states. In figure 3, we plot the frustration ratio (28) as a function of the number of modes. Each point has been numerically obtained by relaxing the energy constraint ($\mathcal{N} \to +\infty$) until the ratio $F^{(n),\mathcal{C}}$ has reached a saturation value $F^{(n)}$ [29]. This corresponds to the limit $\mathcal{C} \to \mathcal{H}$.

3.1. The structure of frustration

In order to try and understand the underlying structure of this frustration, we focus again on qubits and analyze the behavior of the minimum value of the average purity when one requires

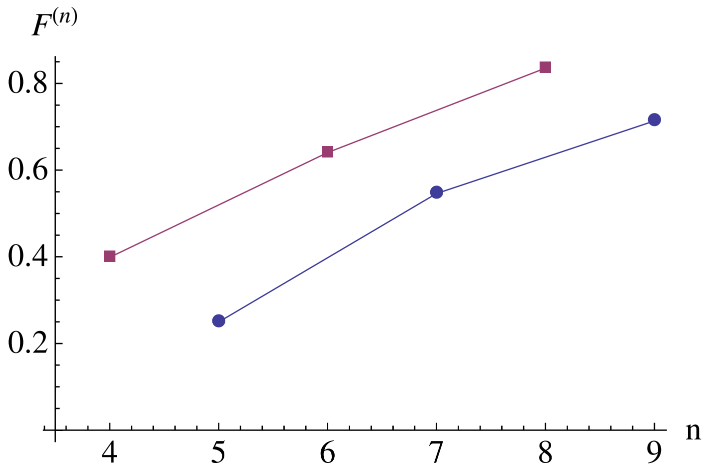

Figure 3. Gaussian states: frustration ratio for and odd (rectangle) and even (circle) number of modes. As explained in the text, each point has been obtained in the saturation regime $\mathcal{C} \to \mathcal{H}$.

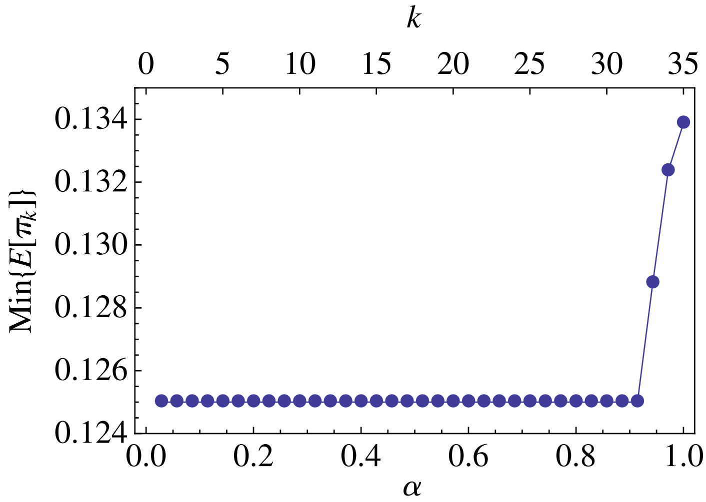

Figure 4. Minimum average purity for $n = 7$ and an increasing number k of bipartitions. Until $k = 32$ all πs are $1/8$ and no frustration appears. For $k = 33$ one partition has purity $\pi = 1/4$. For $k = 34$, two bipartitions yield $\pi = 1/4$. For $k = K = 35$, $\pi > 1/8$ for all bipartitions. $\alpha = k/K$. See figure 5.

the condition (24) for an increasing number k of bipartitions. We proceed as follows: we set $n = 7$, so that the total number of balanced bipartitions is $K = C_3^7 = 35$, and add bipartitions one by one, choosing them so that condition (24) is valid, as far as this is possible. When (24) becomes impossible to satisfy, we require that the average purity be minimal. We plot the minimum average purity as a function of k and $\alpha = k/K$ in figure 4. One observes that it is possible to saturate the minimum $1/N_A = 1/8 = 0.125$ up to $k = 32$ well-chosen partitions. For $k = 33$ all bipartitions yield the minimum $1/8$, except for the last one, which yields $1/4$: frustration appears. For $k = 34$, two bipartitions yield $1/4$. For $k = K = 35$ purity is larger than $1/8$ for *all* bipartitions. Note that the solution with 32 bipartitions at $1/8$ and the remaining *three*

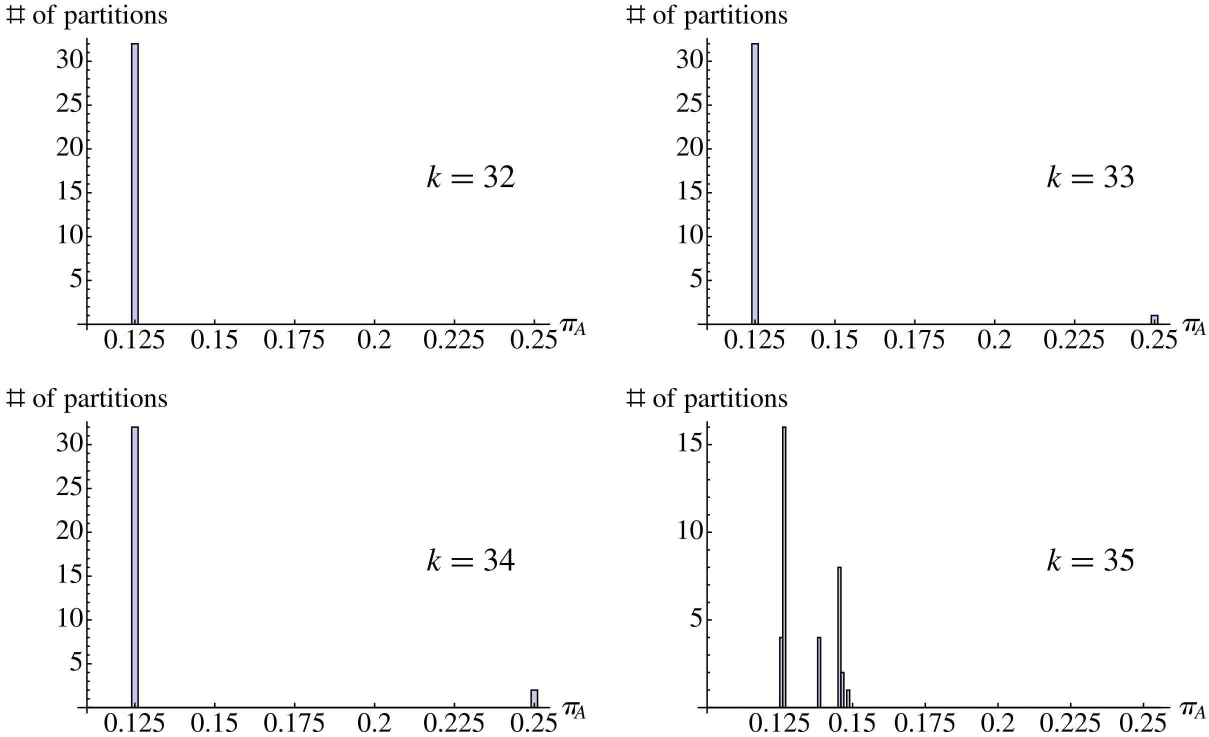

Figure 5. Distribution of purity for $n = 7$ and an increasing number k of bipartitions. See figure 4.

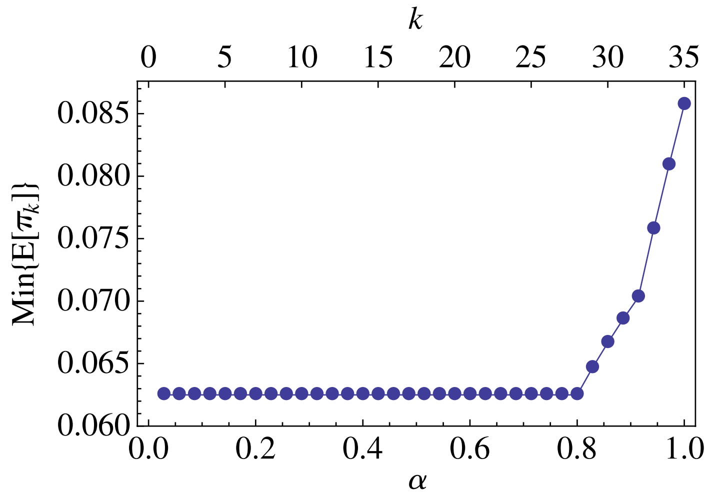

Figure 6. Minimum average purity for $n = 8$ and an increasing number k of bipartitions. Until $k = 28$ no frustration appears. $\alpha = k/K$.

at $1/4$ corresponds to Scott's extremal additive self-dual code and would yield a higher average. The distribution of purity for an increasing number of partitions is shown in figure 5.

The case $n = 8$ is slightly different: see figure 6. Again $K = C_4^8/2 = 35$ (where the factor $1/2$ is a consequence of double counting of partitions when the number of qubits n is even) and there is no frustration up to $k = 28$ bipartitions ($\alpha = 0.8$), if properly chosen (all of them with

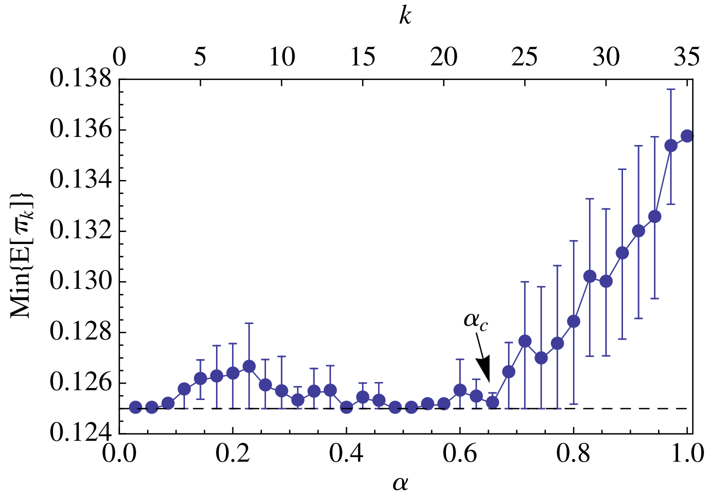

Figure 7. Minimum average purity for $n = 7$ and an increasing number k of randomly selected bipartitions. Every point corresponds to an average over different extractions of k bipartitions. The bars correspond to 68% of the distribution (that can be very asymmetric due to the closeness of the lower bound). $\alpha = k/K$. The average fraction of frustrated bipartitions is $1 - \alpha_c \simeq$ 34%.

a purity $1/16$). When k is further increased, it is no longer possible to reach the lower bound: for $29 \leqslant k \leqslant 32$ the new bipartitions have purity $1/8$. Finally, for $33 \leqslant k \leqslant 35 = K$, the new bipartitions have purity $1/4$.

Another useful test is the extraction of k randomly selected bipartitions and the successive minimization of the average purity. This is a typical test in frustrated systems, e.g. in random [44] and Bethe lattices [45]. In this way one checks the onset of frustration independently of the particular choice of the sequence of bipartitions. In figure 7, we plot the dependence on k and α. Each point corresponds to the extraction of a number of k bipartitions ranging from a few tens to a few hundreds. Frustration appears at rather large values of k, qualitatively confirming the result shown in figure 4. Moreover, we note that for smaller k it is sometimes difficult to reach the minimum. This could be an indicator that for a small number of bipartitions there is a large number of local minima in the energy landscape, which 'traps' the numerical procedure. Note that the curve in figure 7 should monotonically increase as a function of k, so that all deviations from monotonicity are ascribable to the numerical procedure, and are a consequence of the fact that for different values of k, in each run of the simulation, the subset of extracted bipartitions is uncorrelated to the set used for the preceding values of k.

Although the results of this section are not conclusive, they provide a clear picture of the relationship between entanglement and frustration. The latter tends to grow with the size of the system (figures 2 and 3) and it is difficult to study, at least for small values of n, because it appears suddenly at the last few bipartitions (figures 4–6). One estimates, from the results for $n = 7$ qubits in figure 7, an average fraction of frustrated bipartitions $1 - \alpha_c \simeq 34\%$, α_c being a critical ratio.

A posteriori, it is not surprising that multipartite entanglement, being a complex phenomenon, exhibits frustration. It would be of great interest to understand what happens for larger values of n. Different scenarios are possible, according to the mutual interplay between the quantities F and α_c. In particular, the amount of frustration F shows a tendency to increase with n, for both qubit and Gaussian states. This could be ascribed to a decrease of α_c, corresponding to an increasing fraction of frustrated partitions, or to a constant (or even increasing) α_c, corresponding to a constant (or decreasing) fraction of increasingly frustrated bipartitions.

4. Concluding remarks

One important property that we have not investigated here and that is often used to characterize multipartite entanglement is the so-called monogamy of entanglement [14, 46], which essentially states that entanglement cannot be freely shared among the parties. Interestingly, although monogamy is a typical property of multipartite entanglement, it is expressed in terms of a bound on a sum of *bipartite* entanglement measures. This is reminiscent of the approach taken in this paper. The curious fact that bipartite sharing of entanglement is bounded might have interesting consequences in the present context. It would be worth understanding whether monogamy of entanglement generates frustration.

Two crucial issues must be elucidated. The first is that of the striking similarities and small differences between qubits and Gaussian MMES: see table 1 and compare figures 2 and 3. The second is that of the features of MMES for $n \to \infty$. Finally, we believe that the characterization of multipartite entanglement investigated here can be important for the analysis of the entanglement features of many-body systems, such as spin systems and systems close to criticality.

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