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Frustration, entanglement, and correlations in quantum many-body systems

U. Marzolino,[1] S. M. Giampaolo,[2,3] and F. Illuminati[3,4]
[1]*Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany*
[2]*University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria*
[3]*Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, Via Giovanni Paolo II, I-84084 Fisciano (SA), Italy*
[4]*CNISM – Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia, Unità di Salerno, Via Giovanni Paolo II, I-84084 Fisciano (SA), Italy*

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We derive an exact lower bound to a universal measure of frustration in degenerate ground states of quantum many-body systems. The bound results in the sum of two contributions: entanglement and classical correlations arising from local measurements. We show that average frustration properties are completely determined by the behavior of the maximally mixed ground state. We identify sufficient conditions for a quantum spin system to saturate the bound, and for models with twofold degeneracy we prove that average and local frustration coincide.

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Many-body systems are typically modeled by Hamiltonians that are sums of local terms. Each local term operates only on a part of the entire system and acts to minimize the corresponding energy. If different subsystems overlap, the competition among the different local terms can preclude the existence of configurations satisfying all such minimizations simultaneously, a phenomenon known as frustration [1–3]. For classical Hamiltonian systems, frustration is associated to some nontrivial geometric property of the system itself [3]. On the other hand, due to quantum noncommutativity and entanglement [4,5], classically unfrustrated systems may admit frustrated quantum counterparts [4,6–9]. The existence at a qualitative relation between frustration, noncommutativity, and entanglement has motivated recent efforts aiming at qualifying and quantifying frustration in the quantum domain. Frustration criteria, reducing to the Toulouse conditions in the classical case [1], have been introduced recently for systems with nondegenerate ground states [10], and a quantitative relation between a universal measure of frustration and ground-state bipartite entanglement has been established in the form of an exact inequality. However, this specialized result can not be extended straightforwardly to the general case of degenerate ground states due to the fact that different elements of the ground space may exhibit different entanglement properties, and because the ensuing existence of mixed ground states introduces a further ingredient, classical statistical correlations, that may affect frustration at the quantum level.

This work introduces a theory of frustration for quantum systems with arbitrarily degenerate ground states. While including the one discussed in Ref. [10] as a special case, it provides a general picture according to which the interplay between degeneracy and superselection rules results in a highly nontrivial relation between frustration and different types of correlations, classical and quantum. It provides a unified treatment and a rigorous quantification of frustration, expressed in terms of a universal inequality. The latter assesses the relative weights of geometry, bipartite entanglement, and shared classical correlations, identified as the three fundamental sources of frustration in quantum and classical systems. The unified approach is based on the concept of *maximally mixed ground state* (MMGS), that is the statistical mixture with equal *a priori* weights of all possible pure, degenerate ground states. This state always satisfies all the symmetries of the corresponding quantum Hamiltonian and therefore stands as the natural candidate to provide the relevant information on the global characteristics of a quantum system. Thus, the concept of MMGS allows us to introduce a complete classification of many-body quantum Hamiltonians, well beyond the limiting cases discussed in Ref. [10]. Finally, we determine sufficient conditions for the saturation of the inequality that constitute a further quantum generalization of the classical Toulouse criteria.

Let us consider a many-body Hamiltonian $H_T = \sum_S h_S$ sum of local Hamiltonians h_S defined on a finite-dimension subsystem S. Frustration is the impossibility for the ground state ρ_G of the total Hamiltonian H_T to be entirely projected in the ground space of every local Hamiltonian h_S, that is the local ground space. Define then $\rho_S = \mathrm{tr}_R(\rho_G)$, the reduced ground-state density matrix of S, obtained by tracing out all the degrees of freedom of the rest of the system R in ρ_G. A natural way to quantify frustration is to consider the deficiency of the overlap between ρ_G and the projector onto the ground space of the local interactions Π_S [10]:

$$f_S = 1 - \mathrm{tr}(\rho_G \Pi_S \otimes \mathbb{1}_R) = 1 - \mathrm{tr}_S(\rho_S \Pi_S). \qquad (1)$$

This quantity measures how much the global ground state fails to accommodate for the ground states of the local interactions. Here, we should notice, as a side remark, that the fact that f_S depends on the dimension of the ground space appears to agree with the qualitative picture suggested in early attempts to quantify frustration, such as in Ref. [11], where it was noted that, while the presence of geometric frustration strongly affects the energy of a two-dimensional Ising system, its effect is strongly reduced if Ising interactions are replaced by Heisenberg ones. Let us define d as the rank of Π_S, namely, the degeneracy of the local ground space associated to subsystem S. The Cauchy interlacing theorem [12] yields that the universal measure of frustration f_S is bounded from below by the first d largest eigenvalues of ρ_S, arranged in descending order $\{\lambda_i^{\downarrow}(\rho_S)\}_i$ [10]:

$$f_S \geqslant \epsilon_S^{(d)}, \quad \epsilon_S^{(d)} = 1 - \sum_{i=1}^{d} \lambda_i^{\downarrow}(\rho_S). \qquad (2)$$

For pure ground states $\rho_G = |\Psi_G\rangle\langle\Psi_G|$, the quantity $\epsilon_S^{(d)}$ coincides with the distance of ρ_G from the set of states with Schmidt rank D_{Schmidt} less or equal than d [13]. Such distance is an entanglement monotone [13], i.e., a function that vanishes for all separable states and is nonincreasing under local operations and classical communication (LOCC) [14,15]. However, $\epsilon_S^{(d)}$ vanishes also for all entangled states with Schmidt rank $D_{\text{Schmidt}} \leqslant d$ and becomes a faithful entanglement monotone only for $d = 1$ because any entangled pure state has $D_{\text{Schmidt}} \geqslant 2$. Indeed, $\epsilon_S^{(1)}$ coincides with the ground-state bipartite geometric entanglement, defined as the distance of ρ_G from the set of biseparable pure states $|\phi_S\rangle \otimes |\chi_R\rangle$ [16]. On the other hand, the fact that $\epsilon_S^{(d)}$ is not necessarily a full entanglement monotone when $d > 1$ reveals the subtlety of the relation between entanglement and frustration. States in a degenerate global ground space can be entangled just because of the linearity of quantum mechanics, and yet this *a priori* entanglement need not be a source of frustration. An exquisite example is the ferromagnetic spin-$\frac{1}{2}$ Ising model on a triangle. This simple model is obviously frustration free, either classically or quantum mechanically (all local interactions commute). Nevertheless, in the quantum regime, we have that any state of the form $|\psi\rangle = \alpha|\uparrow\uparrow\uparrow\rangle + \beta|\downarrow\downarrow\downarrow\rangle$ is an acceptable ground state that exhibits a nonvanishing entanglement for every possible bipartition as long as $\alpha,\beta \neq 0$. The global ground space is thus doubly degenerate. On the other hand, being the local ground space twofold degenerate as well, for the global ground state it will always be $D_{\text{Schmidt}} \leqslant d = 2$. Regardless of the values of the superposition coefficients, this implies $\epsilon_S^{(2)} = 0$ and therefore the absence of entanglement-induced frustration.

According to Eq. (2), the ground state can belong to three different classes [10]. It will be a *frustration-free* (FF) state if $f_S = \epsilon_S^{(d)} = 0 \; \forall \; S$. It will be an *inequality-saturating* (INES) state if $f_S = \epsilon_S^{(d)} \; \forall \; S$; therefore, an FF state is a particular case of an INES state. Finally, it will be a *non-inequality-saturating state* (non-INES) in all the other situations. As long as the systems being considered admit only one nondegenerate ground state, the same classification applies unambiguously also to the corresponding models. New issues arise if we consider systems possessing different degenerate ground states. In this case, the quantification of frustration provided by Eq. (1) will yield in general state-dependent results within the same class of models and symmetries. For each model, frustration becomes a *local*, state-dependent concept, according to the value taken by Eq. (1) on each different degenerate ground state. On one side, this feature confirms that entanglement is a necessary but not sufficient ingredient to characterize and quantify frustration *globally* in the quantum domain. On the other hand, it implies that the measure defined in Eq. (1) should not be applied separately to each degenerate pure ground state. Rather, it should be evaluated on an appropriate, *average* ground state so defined that it contains all the possible information about the global ground space of the system. In this way, it will be possible to quantify the global frustration properties of the entire model rather than just the ones of a single element of the ground space.

In the following, we will show that identifying the elements, beyond entanglement, that are needed to characterize the global aspects of frustration in the quantum domain also determines the requirements for a state-independent, global quantification of frustration. To this end, the crucial observation is that statistical mixtures of degenerate ground states are themselves legitimate ground states. Moreover, when symmetries are conserved, all the different degenerate ground states have the same statistical possibility to be realized. Therefore, one can introduce as the appropriate *global average* ground state the *maximally mixed ground state* (MMGS), that is the convex combination with equal *a priori* weights of all the possible degenerate ground states. This principle of *a priori* equiprobability guarantees the correct quantification of the global frustration properties of quantum Hamiltonians. The MMGS is the projector on the global ground space (eigenspace of lowest eigenvalue) divided by the degeneracy of this space and, at variance with single pure ground states, it satisfies all symmetries of the Hamiltonian model being considered. We can thus classify the different models and their global frustration properties with respect to the properties of the MMGS: a model is frustration free on average if its MMGS is frustration free; it is INES on average if its MMGS is INES; and it is otherwise non-INES on average if its MMGS is non-INES. If a system admits a unique, nondegenerate ground state, then the local and on-average classifications coincide. In all other cases, if a model is locally FF (INES), then it is also FF (INES) on average, while in general the inverse does not necessarily hold.

When addressing mixed states, the entanglement-to-frustration relation undergoes essential modifications and generalizations. The quantity $\epsilon_S^{(d)}$ ceases in general to be a bipartite entanglement monotone when computed directly on mixed states [17] and must be replaced by its convex roof

$$E_{S|R}^{(d)} = \inf_{\{p_k,|\psi_k\rangle\}} \sum_k p_k \epsilon_S^{(d)}(\mathrm{tr}_R|\psi_k\rangle\langle\psi_k|). \tag{3}$$

In Eq. (3), the infimum is taken over all the possible convex decompositions into pure states $|\psi_k\rangle\langle\psi_k|$ of the total system's ground state: $\rho_G = \sum_k p_k|\psi_k\rangle\langle\psi_k|$. The quantities $E_{S|R}^{(d)}$ and $\epsilon_S^{(d)}$ always coincide for pure states, and in general differ for mixed states. Physically, this difference comes about because the noise present in the reduced density matrix of a globally mixed state is associated not only to the presence of entanglement, as for pure states, but also to the presence of classical statistical correlations that emerge after local generalized measurements on one subsystem [18–20].

Total correlations (quantum plus classical) in mixed states are usually quantified in terms of the von Neumann entropy; however, the relation holds in general: to every entanglement monotone there corresponds a type of classical or quantum correlation emerging when a local generalized measurement is implemented [21]. For our purposes, we need to evaluate the classical correlations between two subsystems, say a and b, in terms of $\epsilon_a^{(d)}$. Although the function $\epsilon_a^{(d)}$ is not a full monotone, it is anyway a proper quantifier of local mixedness, and as such detects correlations between subsystems. Consider then a composite system (made of the subsystems a and b) in a mixed state ρ, and its reduced state $\rho_a = \mathrm{tr}_b\rho$. A generalized measurement on b is defined by a set of positive operators $\{M_b(x)\}$, such that $\sum_x M_b(x) = 1$ [22,23]. The measurement detects the result x with probability $p(x) = \mathrm{tr}(\mathbb{1}_a \otimes M_b(x)[\rho])$, leaving the system in the state $\rho(x) = \frac{1}{p(x)}\mathbb{1}_a \otimes M_b(x)[\rho]$. Replacing the von Neumann entropy with $\epsilon_\alpha^{(d)}$ in the general expression for classical correlations [18,19], one has

$$C_{a|b}^{(d)} = \epsilon_a^{(d)} - \min_{\{M_b(x)\}} \sum_x p(x)\epsilon_a^{(d)}[\mathrm{tr}_b \rho(x)]. \tag{4}$$

The classical correlations $C_{a|b}^{(d)}$ are expressed as the difference between the total correlations $\epsilon_a^{(d)}$, evaluated on the reduced state ρ_a, and the smallest convex combination of total correlations, obtained as the minimum over all possible local generalized measurements $\{M_b(x)\}$ on subsystem b. On the other hand, it is well known that any n-partite mixed quantum state ρ can be obtained from an $(n+1)$-partite pure state by tracing out the degrees of freedom of an ancillary party A. This fact allows us to generalize to the case of the geometric quantity $\epsilon_S^{(d)}$ the results originally obtained for the von Neumann entropy [21], according to the following.

Theorem 1. Purification, entanglement, and classical correlations. Given a pure tripartite state $|\psi_{SRA}\rangle \in \mathcal{H}_S \otimes \mathcal{H}_R \otimes \mathcal{H}_A$ and its reduced density matrices $\rho_{SR} = \mathrm{tr}_A|\psi_{SRA}\rangle\langle\psi_{SRA}|$, $\rho_{SA} = \mathrm{tr}_R|\psi_{SRA}\rangle\langle\psi_{SRA}|$, and $\rho_S = \mathrm{tr}_{RA}|\psi_{SRA}\rangle\langle\psi_{SRA}|$, then

$$\epsilon_S^{(d)} = E_{S|R}^{(d)} + C_{S|A}^{(d)}, \tag{5}$$

that is, the total correlations expressed by the geometric quantity $\epsilon_S^{(d)}$ are the sum of the bipartite entanglement (convex roof) between S and R and the classical correlations between S and A. The proof of the theorem is provided in the Supplemental Material [24]. We will apply Theorem 1 to the purification of the MMGS with the ancilla A, where the presence of classical correlations detected by local generalized measurements on A is a consequence of the degeneracy of the ground state. Conceptually, the ancillary party A can be thought of as a suitable quantum reservoir entangled with the bipartite system $(S|R)$, yielding the MMGS as the on-average reduced equilibrium state [25]. Equivalently, A can be seen as a quantum reference system, such that if one traces over A, every ground state of $(S|R)$ is equiprobable, as identified by a complete set of superselection rules [26].

Comparing Eqs. (5) and (2), we obtain a unified lower bound to frustration encompassing both the nondegenerate and degenerate cases:

$$f_S \geqslant E_{S|R}^{(d)} + C_{S|A}^{(d)}. \tag{6}$$

The above exact inequality yields that, in the quantum domain, frustration is not only due to the underlying geometry, as for the classical case, and/or to entanglement, as for systems with nondegenerate ground states. In general, it depends on the interplay of these two elements with a third source, namely, statistical correlations established outside of the d-fold-degenerate local ground space due to the degeneracy encoded in the MMGS. When the ground state is pure and nondegenerate, the general bound Eq. (6) evaluated on the MMGS reduces to Eq. (2), as the classical correlations $C_{S|A}^{(d)}$ vanish and the convex roof $E_{S|R}^{(d)}$ coincides with $\epsilon_S^{(d)}$.

Let us illustrate with a simple but nontrivial example the difference between the local and on-average characterizations of frustration provided, respectively, by Eqs. (2) and (6). Consider a ring of five spins with periodic boundary conditions described by a ferromagnetic Ising Hamiltonian $H = -\sum_{i=1}^5 S_i^x S_{i+1}^x$ ($S_6^\alpha \equiv S_1^\alpha\ \forall\ \alpha = x,y,z$). All local terms in the Hamiltonian commute: in this sense, the model is classical. The global and local ground states are both twofold degenerate (spin-flip symmetry). Since every element of the global ground space is FF, the model is locally always FF, i.e., FF on each of the different degenerate global ground states, and hence FF on average, that is FF on the MMGS. Next, let us modify the Hamiltonian from classical Ising to quantum XY: $H = -\sum_{i=1}^5 (S_i^x S_{i+1}^x + \Delta S_i^y S_{i+1}^y)$, while the geometry of the system remains unchanged. One would now expect that frustration in the system should arise from the noncommutativity of the local terms in the XY Hamiltonian (now the local ground-space degeneracy $d = 1$). Accordingly, one verifies that the model is INES on average, i.e., the inequality (6) is saturated by the MMGS, with the actual values of the frustration measure f_S and of the total correlations $\epsilon_S^{(1)}$ depending on the anisotropy Δ. For instance, for $\Delta = 0.1$, one has $f_S \equiv \epsilon_S^{(1)} \simeq 0.476$ for each of the five different spin pair-interaction terms. However, regardless of the value of Δ, such a model is never locally INES. Indeed, given the doubly degenerate global ground space, let us pick, e.g., the ground state that is an eigenstate of the parity operator along the x direction with eigenvalue $+1$. For this pure ground state, the measure of frustrations f_S takes always the same values as for the MMGS (this is actually an interesting general property for all twofold-degenerate ground states [24]). However, the bipartite geometric entanglement $E_{S|R}^{(1)}$ is always well below the total correlations $\epsilon_S^{(1)}$. For instance, with $\Delta = 0.1$, one has $E_{S|R}^{(1)} \simeq 0.001 \ll \epsilon_S^{(1)} \simeq 0.476$. The impossibility to saturate inequality (2) is related to the fact that the selected pure ground state breaks the symmetry of the model Hamiltonian. Modifying the geometry, e.g., by adding a direct antiferromagnetic interaction between the first and the third spins: $H' = S_1^x S_3^x + \Delta S_1^y S_3^y$ introduces a further, geometric source of frustration. In this case, the MMGS no longer saturates inequality (6) and the system ceases to be INES, thus signaling the presence of geometric frustration.

From the above discussions it follows that it would be desirable to identify a set of conditions to detect *a priori* the frustration properties of the global ground space of a given model or class of models. These conditions should include as a particular case the ones previously determined for nondegenerate ground states [10]. Extending the Toulouse criteria [1] to the quantum domain, we need to identify a *prototype* model that is INES on average and then define a group of local operations under which the property of being INES on average is preserved. We define the prototype model as follows.

Prototype model. A quantum spin Hamiltonian of the type

$$H = \sum_{ij} h_{ij} = -\sum_{ij,\mu} J_{ij}^\mu S_i^\mu S_j^\mu \tag{7}$$

is a *prototype* model if there exists at least one local ground space common to all pair local interactions h_{ij} and every local coupling vector $\vec{J}_{ij}$ has non-negative components. Having defined the prototype model, we state the following:

Conjecture 1. INES property and prototype models. All prototype models are INES on average.

Conjecture 2. INES property and local transformations. Every model obtained from a prototype model by local unitary operations on each spin and partial transposition on any arbitrary set of sites $\{K\}$ is still INES on average.

It is evidently quite hard to prove these two conjectures in all generality. In the Supplemental Material [24], we provide an analytical proof for the one-dimensional quantum XY model in the thermodynamic limit, and strong numerical evidence obtained for more than 2×10^5 randomly generated models with exchange interactions on arbitrary random graphs with a total number of sites $N \leqslant 9$. Preservation of the INES property on average under partial transposition is to be expected because this property is directly related to the absence of geometric frustration in the model. Nevertheless, the preservation of the INES property on average is far from trivial. Indeed, contrary to what happens under local unitary transformations, the properties of degenerate ground states of a given Hamiltonian *before* and *after* partial transposition need not be related. As a straightforward example, let us consider a spin-$\frac{1}{2}$ Heisenberg chain (open boundary conditions) of $N = 4$ spins with homogeneous nearest-neighbor ferromagnetic couplings. The global ground state is fivefold degenerate while the local ground space is threefold degenerate, and for any couple of interacting spins we have $f_S = \epsilon_S^{(3)} = 0$. Performing partial transposition on spins 2 and 4 (or, equivalently, on spins 1 and 3) the original model maps in an antiferromagnetic Heisenberg chain possessing both a nondegenerate global and local ground state with $f_S = \epsilon_S^{(1)} \simeq 0.067$ for both the pairs of spins (1,2) and (3,4), while $f_S = \epsilon_S^{(1)} = \frac{1}{2}$ for the pair of central spins (2,3). The transformed model has very different ground-state properties compared to the initial one, and yet it remains INES.

In conclusion, we have derived an exact lower bound on a universal measure of frustration in the general case of degenerate ground states. The bound is expressed as the sum of two contributions, one due to bipartite ground-state entanglement and one due to bipartite classical correlations that are established after local generalized measurements on a quantum reservoir or a quantum reference frame. This further source of frustration adds to geometry and entanglement, yielding a rather complex structure that involves several fundamental concepts of quantum physics: entanglement of mixed ground states, classical correlations arising from quantum degeneracy, and the purification of ground states via quantum reservoirs or quantum reference frames.

We have showed that the frustration properties of quantum many-body Hamiltonians are encoded in the maximally mixed ground state (MMGS), that is the convex combination with equal coefficients of all the degenerate pure ground states. Given such on-average, global classification, we have determined the sufficient conditions for a quantum spin system to achieve the bound, generalizing the results obtained in the case of models with nondegenerate ground states [10]. For systems with doubly degenerate ground states we have proved rigorously that local and average frustration coincide: all degenerate ground states, and therefore also the MMGS, exhibit the same frustration properties [24].

The fact that the residual classical correlations after local generalized measurements are identified as a novel source of frustration in quantum many-body systems may open interesting research insights concerning competitions among quantal and nonquantal aspects in Hamiltonian spin dynamics, as in the case of the anisotropic Heisenberg models in an external field, or competition between quantal dynamics and thermal fluctuations. Future investigations should address the role that the presence or absence of the INES property on average actually plays in computational [27], information-theoretic [28–31], and thermodynamic characterizations [32,33] of many-body quantum systems. Experimental consequences might soon be derived and tested, as the controlled quantum simulation of spin systems, classical and quantum, is rapidly progressing, from the first demonstration of antiferromagnetic spin chains with optical lattices [34] and of classically frustrated Ising spins with trapped ions [35] and with optical lattices [36] to the very recent comprehensive proposals for the quantum simulation of large classes of frustrated quantum spin models with ion crystals [37] and color centers in diamond [38], which should open the way in the near future to the precise verification of long-standing predictions on exotic phases of matter. In this respect, the use of conceptual and technical tools inspired by quantum information and entanglement theory can yield broader and deeper understanding [39] of collective and complex quantum phenomena beyond the traditional Landau-Ginzburg framework of quantum phase transitions based on symmetry breaking and local order parameters.

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