Characterizing and Quantifying Frustration in Quantum Many-Body Systems

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We present a general scheme for the study of frustration in quantum systems. We introduce a universal measure of frustration for arbitrary quantum systems and we relate it to a class of entanglement monotones via an exact inequality. If all the (pure) ground states of a given Hamiltonian saturate the inequality, then the system is said to be inequality saturating. We introduce sufficient conditions for a quantum spin system to be inequality saturating and confirm them with extensive numerical tests. These conditions provide a generalization to the quantum domain of the Toulouse criteria for classical frustration-free systems. The models satisfying these conditions can be reasonably identified as geometrically unfrustrated and subject to frustration of purely quantum origin. Our results therefore establish a unified framework for studying the intertwining of geometric and quantum contributions to frustration.

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Frustration consists in the impossibility of determining configurations that minimize simultaneously the energy of competing interactions [1–3]. In recent years it has been realized that classically unfrustrated systems can have frustrated quantum counterparts [4–7]. Indeed, in the quantum case, additional sources of frustration may arise due to noncommutativity and entanglement [5,8]. Hence, although the notion of frustration has often been considered from the perspective of statistical physics, in the quantum domain interesting novel phenomena take place even in the presence of few entangled elements [5,8,9]. It is however far from clear how to distinguish geometric from purely quantum frustration and whether the distinction is free of ambiguities. To the best of our knowledge this issue has never been addressed. Moreover, despite frustration being a well-defined and intuitive concept, a measure for quantum systems which fully captures all its aspects is still lacking. Existing proposals for quantifying frustration in quantum systems focus on particular aspects of the phenomenon. Some proposals are based on classical equivalents of a given quantum system [10], making it impossible to recover information about quantum correlations. Others apply only in the thermodynamic limit [11,12], or on the competition between local and nonlocal interactions from a purely quantum perspective [5], thus making it challenging either to study finite-size systems or to understand the transition to classically frustrated systems. The need for a systematic investigation of this issue at a foundational level is thus quite compelling. Even more so, as quantum simulators of classical as well as quantum frustrated magnetic systems, at least in the simplest Ising and J_1-J_2 cases, are being demonstrated with ultracold atoms in optical lattices [13,14] and trapped ions [15], or proposed, e.g., with cold Coulomb crystals [16]. Furthermore, such an investigation would be of great help and guidance for the design of entanglement-based numerical simulations of frustrated quantum spin models [17].

The aim of this work is to introduce a universal measure of frustration for quantum systems and define a unified framework suitable to understand the intertwining of the geometric and quantum contributions to frustration. To this end we focus on the microscopic properties of finite-size models from a purely quantum perspective without resorting to semiclassical approximations. After introducing a universal measure of frustration, we prove that it is an upper bound to a class of entanglement monotones that in particular cases reduces to the bipartite geometric entanglement. We then establish sufficient conditions for a quantum spin system to saturate the bound and support them with extensive strong numerical evidence. Finally, we show how these conditions essentially generalize to the quantum domain the Toulouse criterion for frustration-free classical systems.

Consider a system in a pure state $\rho = |\psi\rangle\langle\psi|$, and let Π be the projector onto a given subspace. Then

$$f = 1 - \mathrm{tr}[\rho\Pi], \tag{1}$$

quantifies how much ρ fails to fully overlap with the subspace selected by Π. Let now $\rho = |G\rangle\langle G|$ be the ground state (GS) of a many-body system $H = \sum_S h_S$ and Π_S the projector onto the GS of the local interactions h_S corresponding to subsystem S. Then $f_S = 1 - \mathrm{tr}[\rho\Pi_S]$ is a well-defined and unambiguous measure of the frustration of h_S. On the other hand, denoting by R the rest of the system, consider the following entanglement monotone:

$$E^{(d)}(S|R) = 1 - \sum_{i=1}^{d} \lambda_i^{\downarrow}(\rho_S), \tag{2}$$

where $\lambda_i^{\downarrow}(\rho_S)$ are the eigenvalues of $\rho_S = \mathrm{tr}_R\rho$ in decreasing order and $d < \dim[\mathcal{H}_S]$, with $\mathcal{H}_S$ the Hilbert space of

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S. Notice that $E^{(d)}(S|R) = E^{(d)}(R|S)$. The right-hand side of Eq. (2) vanishes only on states with a Schmidt rank smaller or equal than d [18]; for $d = 1$ it reduces to the bipartite geometric entanglement, defined as the distance from the set of biseparable states [19]. Fix now d to be the degeneracy of the local interaction h_S (i.e., Π is rank-d). Then, by the Cauchy interlacing theorem (see also Lemma 1 in the Supplemental Material [20]) it follows that

$$f_S \geq E_S^{(d)}, \tag{3}$$

where $E_S^{(d)} \equiv E^{(d)}(S|R)$ is the distance from $|G\rangle$ to the closest state with Schmidt rank $r \leq d$ [18].

Despite its apparent simplicity, Eq. (3) has the remarkable feature of directly relating frustration to entanglement. This quantitative relation holds for any pure state ρ and any interacting quantum system and hence is universal. Actually, Eq. (3) holds as well for any mixed state, although in this case $E_S^{(d)}$ is no longer an entanglement monotone. An immediate consequence of Eq. (3) is that the frustration-free condition, $f_S = 0\ \forall\ S$ is a bound on the maximum Schmidt rank of the global ground state $|G\rangle$. For interactions h_S with nondegenerate local GSs $|G_S\rangle$, $d = 1\ \forall\ S$, this implies the separability of the global GS in the tensor product of the local GSs: $|G\rangle = \bigotimes_S |G_S\rangle$. That the absence of frustration should be related to some form of factorization of the GS had already been observed, at a semiquantitative level, for models in transverse fields [6]. On the other hand, saturation of the inequality, $f_S = E_S^{(d)}$ for some S, imposes a block-diagonal form of the reduced state ρ_S, with eigenvalues $\lambda_i^{\downarrow}(\rho)$, $i = 1, \ldots, d$ corresponding to the block spanned by Π (see Lemma 1 in [20]). Hence ρ_S cannot exhibit coherence between the lowest and excited energy levels of h_S: the largest contribution to ρ_S must come from the local ground subspace.

Summarizing the above discussion, we can state that a GS $\rho = |G\rangle\langle G|$ of a many-body Hamiltonian of the form $H = \sum_S h_S$ is a frustration-free (FF) state if and only if $f_S = 0\ \forall\ S$, and is an inequality saturating (INES) state if and only if $f_S = E_S^{(d)}\ \forall\ S$. Clearly, a FF state is also an INES state. A Hamiltonian H is then a FF Hamiltonian if all its GSs are FF states, and is an INES Hamiltonian if all its GSs are INES states. In general, it is easy to show that states with at least one $f_S > 0$ have higher energy compared to the corresponding FF state. Hence, if a model is globally degenerate and one global GS is a FF state, then this is true for all other GSs. Unlike the FF property, the INES property is not universal; i.e., it does not necessarily apply to all the GSs of a system. This is due to the fact that unlike the FF property, the INES property does not specify the GS energy. Total frustration F can then be defined by averaging over all the local measures f_S.

We will now exploit Eq. (3) to generalize the classical criteria for the absence or presence of frustration to the quantum domain and to understand the intertwining of geometric and purely quantum contributions to frustration. According to Toulouse [Formulation 1]: A classical Hamiltonian H is frustrated if and only if it is impossible to transform H into a fully ferromagnetic Hamiltonian by means of local spin inversions. This occurs only when a closed loop exists with an odd number of antiferromagnetic interactions [1,2,4]. Indeed, the Toulouse criterion computes exactly the parity of antiferromagnetic bonds on a closed loop, according to [Formulation 2]: For a given Hamiltonian a loop is frustrated if the quantity $P = (-1)^{N_{af}} = -1$, where N_{af} is the number of antiferromagnetic bonds. Next, consider the simplest quantum extension of classical models, the quantum Ising model $H = \sum_{i<j} J_{ij} S_i^z S_j^z$ ($d = 2$). Clearly, the model is unfrustrated if the GS is of the form $|\psi\rangle = \bigotimes_{i=1}^N (S_i^x)^{\gamma_i} \times (\alpha|\uparrow\uparrow\cdots\rangle + \beta|\downarrow\downarrow\cdots\rangle)$, with $\gamma_i = 0, 1$. Indeed, in this case $f_{ij} = E_{ij}^{(2)} = 0\ \forall\ S \equiv ij$, and Eq. (3) is saturated by all GSs. On the contrary, if the model is frustrated there exists at least one GS which is not an INES state. In fact, all separable GSs exhibit $E_{ij}^{(2)} = 0$ on all pairs and $f_{ij} > 0$ on at least one pair. Therefore, in terms of Eq. (3), the immediate extension to the quantum Ising case of the Toulouse condition is [Formulation 3]: A quantum Ising Hamiltonian is frustrated if and only if it is not an INES model. Although the Ising model does not contain quantum features, such as noncommutativity of the local interactions, and therefore can only exhibit geometric frustration, the possibility of restating Toulouse criterion in terms of f and an entanglement monotone $E_S^{(2)}$ is remarkable as it provides the first bridge between the classical and the quantum domains.

From the Ising example we learn that in the quantum domain the relevant information to detect frustration is the existence of GSs not being INES states, rather than that of GSs not being FF states. This is because for quantum systems frustration arises not only from topological constraints (so-called geometric frustration) but as well from purely quantum ones. Consider the following classically unfrustrated Heisenberg Hamiltonian for four spins on an open chain: $H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$, where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$, $d = 1$ and the global GS of H is nondegenerate. The quantum version of this model is frustrated, as in the GS the total measure of frustration $F = N^{-1}\sum_{ij} f_{ij} = \frac{1}{6}(3 - \sqrt{3})$, where $N = 3$ is the number of bonds. Remarkably, the frustrated GS is an INES state;, hence, the frustrated model is still an INES model, in contrast to what occurs in the Ising case. Let us now add to H some geometric frustration, i.e., $H' = H + \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$. Now one has $f_{ij} = 2/5 > E_{ij}^{(1)} = 1/3\ \forall\ (ij)$, and hence the frustrated GS is not an INES state. Indeed, the Ising model can only exhibit geometric frustration, even in its quantum version, as the local GSs are always unentangled. On the contrary, the GS of each Heisenberg local pair term is a maximally entangled Bell state. Accordingly, the model can either be an INES model or not, depending on the topology of the system. Actually, even if geometric frustration is absent, yet monogamy of entanglement [21] prevents the global GS from minimizing all the local terms, and the model is both frustrated and INES. This strongly suggests that failure to saturate Eq. (3) is a signature of the presence of geometric frustration.

From the above discussion it follows that it would be highly desirable to identify conditions detecting *a priori* the nature of the frustration in a given quantum system. Considering hereafter only models with nondegenerate global GS, we approach the problem by observing that the classical Toulouse condition contains two main ingredients: a ferromagnetic model, which serves as the prototype of FF models, and a gauge group under which the FF property is preserved. We thus look for a prototype INES model and a gauge group under which the INES property is preserved. To fix the stage, consider the general XYZ (Heisenberg) exchange Hamiltonian

$$H = \sum_{ij} h_{ij} = -\sum_{ij,\mu} J_{ij}^{\mu} S_i^{\mu} S_j^{\mu}, \qquad (4)$$

where $\mu = x, y, z$, with coupling vectors $\vec{J}_{ij} = (J_{ij}^x, J_{ij}^y, J_{ij}^z)$ on arbitrary graph geometries.

Prototype model.—A nondegenerate quantum Hamiltonian as in Eq. (4) will be called a prototype if (1a) there exists at least one local GS common to all local pair interactions h_{ij}'s, and (1b) each local coupling vector $\vec{J}_{ij}$ has non-negative components (i.e., it is a full ferromagnet: $J_{ij}^{\mu} \geq 0 \ \forall \ i, j, \mu$ and there exists a common two-body state vector $|\phi\rangle$ which is ground state of all h_{ij}). [*Conjecture 1.*]: All prototype models are INES.

Note the remarkable parallelism between condition (1a) and the FF condition, which essentially requires the existence of at least one global GS common to all h_{ij}'s. From our conjecture, it follows that if $d = 1$ then all h_{ij}'s must admit the same Bell state as GS. Since the GS of a given h_{ij} with positive $\vec{J}_{ij}$ is determined by the lowest value component of the vector, it follows that it must be along the same axis for all $\vec{J}_{ij}$ in the prototype model. Any model obtained from the prototype by means of tensoring local unitary operations is clearly still an INES model with the same set of f_{ij} and $E_{ij}^{(d)}$'s. In fact, one has [*Conjecture 2.*]: Any model $H' = H^{T_K}$ which can be obtained from a prototype model H by partial transposition on any set of sites K is still an INES model.

Applying partial transposition [22] to a prototype Hamiltonian changes f_{ij} and $E_{ij}^{(d)}$; however, saturation of Eq. (3) is preserved. Although an analytical proof of these conjectures appears challenging, in the Supplemental Material [20] we provide compelling numerical evidence of their validity. This is a very significant result, as it implies that not only local rotations but also partial transpositions do preserve the INES property. It is not *a priori* obvious that this would be the case, since, as already noted, both sides of inequality (3) are typically changed by a partial transposition. Indeed, partial transposition is intimately related to parity, as $P_k(H) = S_k^y H^{T_k} S_k^y$, where P_k is the parity transformation on site k [$P(\mathbf{S}) = -\mathbf{S}$]. Thus, according to Conjecture 2, the local gauge group is $G = SU(2) \otimes \mathbb{Z}_2$. An element of $SU(2)$ acting on S^{μ} is represented by a transformation $R \in SO(3)$, whereas a parity transformation is simply $-\mathbb{1}$. Hence, spin operators transform according to the $O(3)$ representation of G, and a local gauge transformation $\mathfrak{g} = \bigotimes_i g_i$ (with $g_i \in G$) maps two-body interactions $\sum_{\mu\nu} J_{ij}^{\mu\nu} S_i^{\mu} S_j^{\nu}$ into $\sum_{\mu\nu} [R_i^{\top} J_{ij} R_j]^{\mu\nu} S_i^{\mu} S_j^{\nu}$. Given a general XYZ Hamiltonian $H = -\sum_{ij}\sum_{\mu} J_{ij}^{\mu} S_i^{\mu} S_j^{\mu}$, we derive necessary and sufficient conditions for H to be equivalent to a prototype model under the action of some $\mathfrak{g} \in G^{\otimes N}$. Consider two sites a and b and let $p(a \to b) = \{(a, i_1), (i_2, i_3), \ldots, (i_k, b)\}$ be any path from a to b, where all pairs $(i, j) \in p$ interact. Define the sign of the path p as

$$\pi(p(a \to b)) = \prod_{(i,j)\in p} \mathrm{diag}(s_{ij}^x, s_{ij}^y, s_{ij}^z), \qquad (5)$$

where $s_{ij}^{\mu} = \mathrm{sgn}(J_{ij}^{\mu\mu})$ and we define $\mathrm{sgn}(0) = 1$, with the product taken over all adjacent pairs ij belonging to the path $p(a \to b)$. Note that $\pi(p(a \to b)) = \pi(p(b \to a))$. We state the following. [*Theorem*] Necessary and sufficient conditions for a Heisenberg Hamiltonian H to be mapped into a prototype model by a local gauge transformation are (2a) All coupling vectors $\vec{J}_{ij}$, have the smallest absolute value component along the same axis; (2b) For any pair of spins a and b, $\pi(p(a \to b))$ is independent of the path p from a to b. As shown in the Supplemental Material [20], condition (2b) guarantees that the system can be brought to a fully ferromagnetic system. When this condition is met, the dependence of π on the path can be dropped. Then one can consider $\pi(a \to b)$ as a "conservative field" which dictates the local transformation that has to be applied in b so that the sign of any path from a to b is positive. If this holds for all b, one can turn all the couplings to positive by means of local transformations. On the other hand, condition (2a) is related to the existence of the same Bell state as the common ground state of all the two-body interactions. A remarkable simplification occurs when the system is translationally invariant. In that case: [*Theorem*] If a model satisfies $\pi(\ell) = +\mathbb{1}$, for every loop ℓ in the elementary cell and all coupling vectors have the smallest component along the same axis, then it is an INES model (Proof in the Supplemental Material [20]). This theorem encodes in compact form three of Toulouse's criteria, one for each spatial direction. This strongly suggests that the class of INES models defined by conditions (2a) and (2b) can be identified as that of geometric frustration-free spin-$1/2$ quantum models. Our analysis reveals that the quantum nature of the model affects the very notion of geometric frustration. Condition (1a) or equivalently (2a) is a consequence of the existence of three inequivalent ferromagnetic states, i.e., the triplet states. This constraint, however, is only relevant in systems with inhomogeneous couplings. Otherwise, conditions (2a) and (2b) simply reduce to a generalized form of Toulouse's criterion. Being the class of geometric frustration-free quantum systems more restrictive than its classical analogue, one may expect that further investigation reveals generic properties which so far failed to be properly generalized.

On the other hand, the class of geometric unfrustrated quantum systems is strictly larger than that of frustration-free systems. A deeper investigation of geometric FF quantum models might thus unveil several relevant applications. For example, the largest eigenvalues of ρ_{ij} identified by Π_{ij} may provide guidelines for designing optimal entanglement renormalization algorithms and other tensor network ansatz [23]. Moreover, the measure of frustration that we have introduced and its relation to geometric entanglement is not restricted to local two-body Hamiltonians or spin-$1/2$ systems and might be exploited to gain understanding of geometric frustration in arbitrary quantum many-body systems.

According to our results, the INES class of models is larger than that of geometric FF models, thus suggesting that the INES property has deeper implications than merely detecting the presence or absence of geometrical frustration. For example, the fact that INES geometrically frustrated models may behave differently from non-INES geometrically frustrated ones hints at a significant role of the INES property as a diagnostic tool for quantum phase transitions in complex and frustrated models. Indeed, consider a frustrated system such as the elementary cell of the pyrochlore lattice $H = J(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_3 \cdot \mathbf{S}_4) + (\mathbf{S}_1 + \mathbf{S}_2) \cdot (\mathbf{S}_3 + \mathbf{S}_4)$ [24]. For $J > 1$ the system is INES since it is in a dimer phase and all dimers have $f = E^{(1)} = 0$, whereas all other bonds are in a maximally mixed state, hence $f = E^{(1)} = 3/4$. Exact diagonalization shows that the transition from the dimer ($J > 1$) to the plaquette phase ($0 < J < 1$) corresponds to the transition from INES to non-INES, with $f_{12} = f_{34} = 1 > E^{(1)}_{12} = E^{(1)}_{34} = 2/3$. This suggests a correspondence between the different quantum phases of a frustrated model and its INES or non-INES character. Indeed, the relation between geometric frustration and exotic matter phases was previously pointed out in [11]. One may also ask how the presence (absence) of geometric frustration and the INES (non-INES) nature of a system gets reflected in computational [25], information-theoretic [10,26] or thermodynamic terms [12]. Necessary steps toward further investigation of all these open fundamental questions will require achieving a rigorous mathematical control and understanding of our quantum Toulouse conditions as well as the generalization of our approach to globally degenerate systems. Although some instances of degeneracy can be easily accommodated within our scheme (e.g., odd number of spins), some others (e.g., thermodynamic degeneracy) are still elusive, but in very simple cases such as the XY model.

The essential and intriguing role played by partial transposition cannot go unnoticed. The fact that the prototype models preserve their INES character under partial transposition is to be expected if INES has anything to do with the presence or absence of geometric frustration. Nevertheless, the preservation of the INES property is far from trivial because, unlike with the case of local unitary transformations, the GSs of a Hamiltonian before and after partial transposition are not immediately related. Indeed, we expect that the rigorous proof of our conjectures will shed further light on the role played by partial transposition and its relation to geometric frustration. From a directly physical point of view, as already noticed, our quantitative analysis confirms previous evidence [6] that some form of factorization of the global GS is a necessary ingredient in the characterization of FF systems. It is tempting to speculate that investigating the intertwining between frustration and factorizability of higher order (k separability, including dimerization and trimerization) could lead to a unified framework for the understanding of the relations between frustration, the role of hierarchical geometric entanglement [19] in collective quantum phenomena, and the characterization of entanglement and k separability by local unitaries [27].

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