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Characterizing and quantifying quantum frustration: relations to entanglement and correlations, exact bounds, and local and global observables

We discuss a general scheme for the study of frustration in quantum systems. We introduce a universal measure of frustration for arbitrary quantum systems with Hamiltonians made of sums of local two-body contributions in terms of the overlap between the unfrustrated ground state of the pair Hamiltonians and the frustrated ground state of the total Hamiltonian. We derive an exact lower bound this overlap measure of frutration 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. If all the (pure) ground states of a given Hamiltonian saturate the inequality, then the system is said to be inequality saturating. 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. The mathematical scheme can be put to test by relating the overlap measure and the inequalities it obeys to global and local observables in terms of the static structure factor and transverse n-point correlation functions.

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