Probing Quantum Frustrated Systems via Factorization of the Ground State

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The existence of definite orders in frustrated quantum systems is related rigorously to the occurrence of fully factorized ground states below a threshold value of the frustration. Ground-state separability thus provides a natural measure of frustration: strongly frustrated systems are those that cannot accommodate for classical-like solutions. The exact form of the factorized ground states and the critical frustration are determined for various classes of nonexactly solvable spin models with different spatial ranges of the interactions. For weak frustration, the existence of disentangling transitions determines the range of applicability of mean-field descriptions in biological and physical problems such as stochastic gene expression and the stability of long-period modulated structures.

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Introduction.—Interest in frustrated quantum systems is due to the fact that they exhibit a large ground-state degeneracy, or quasidegeneracy, associated with complex structures of the quantum phase diagrams [1]. Moreover, frustrated spin models arise naturally in a variety of physical situations, e.g., in the study of high-T_c superconductivity [2,3], long-period modulated structures of condensed matter [4], and biological systems with stochastic components [5]. Unfortunately, rigorous results are available so far only for ultrasimplified models [1], while numerical simulations are challenging, as quantum Monte Carlo methods are not practical for frustrated spin and fermion models [6], and the density matrix renormalization group is difficult to apply to systems with dimensionality larger than 1 and/or periodic boundary conditions [7]. Furthermore, criteria to quantify frustration and the classification of "weakly" and "strongly" frustrated systems have been mainly phenomenological, with little or no rigorous physical and mathematical insight [8].

Recently, a method based on quantum information techniques [9] has allowed us to establish rigorously that large classes of (generally nonexactly solvable) frustration-free quantum spin models admit totally disentangled ground states (GS) at finite values of the interaction strengths and of the external fields [10]. These factorized GS coincide exactly with the mean-field solutions and identify well-defined magnetic orders endowed with simple spatial periodicities. In this Letter we build on that formalism to investigate the physics of quantum frustrated systems by showing that GS separability is a measure of quantum frustration that discriminates quantitatively regimes of weak and strong frustration. Indeed, we prove the existence of a critical frustration threshold below which fully factorized GS are allowed and correspond to definite magnetic orders with simple periodicity for quantum spin models belonging to different universality classes and with different types and ranges of interactions. We then prove rigorously the existence of disentangling transitions in the GS in the regime of weak frustration and identify the different magnetic orders and their quantum phase boundaries. That, indeed, entanglement and separability can be used to qualify and quantify frustration (and vice versa) can be intuitively understood by observing that the presence of frustration tends to enhance correlations among the constituents and thus to depress the possibility for the occurrence of separable (uncorrelated) states. We also discuss some predictive consequences of these results on the study of complex systems in physics and biology. Although in what follows, for ease of presentation, the analysis is carried out in detail for one-dimensional systems, it is straightforward to extend it and apply it in general to systems of arbitrary dimensionality.

We consider spin-$\frac{1}{2}$ systems for which frustration arises from the simultaneous presence of competing antiferromagnetic exchange interactions of different spatial range. The anisotropy $J_\alpha \geq 0$ ($\alpha = x, y, z$) in the spin-spin coupling at sites i and j of the lattice with distance $r = |i-j|$ is taken independent of r, and all couplings are rescaled by a common, distance-dependent factor $f_r > 0$. The general model Hamiltonian then reads

$$H = \sum_{i,r\leq r_{\max}} f_r (J_x S_i^x S_{i+r}^x + J_y S_i^y S_{i+r}^y + J_z S_i^z S_{i+r}^z) - h \sum_i S_i^z, \tag{1}$$

where S_i^α are the spin-$\frac{1}{2}$ operators at site i; h is the external magnetic field; and $r_{\max} > 1$ is the interaction range, i.e., the maximum distance between two spins with nonvanishing coupling. Without loss of generality we assume $J_x \geq J_y$. This general XYZ Hamiltonian with interactions of arbitrary range includes as subcases many different models spanning several classes of universality, such as the short- and long-range Ising, Heisenberg, XY, XX, and XXZ models. We first recall briefly the basic findings on GS factorization in frustration-free spin models [10]. The quantity controlling GS factorization is the entanglement excitation energy (EXE) ΔE [9]. At every site k it is defined as $\Delta E = \min_{\{U_k\}}\langle G|U_k H U_k|G\rangle - \langle G|H|G\rangle$. Here $|G\rangle$ is the GS of the system and U_k is any local rotation acting on the spin at site k, i.e., a single-spin unitary operation [9]: $U_k \equiv \bigotimes_{i\neq k}\mathbf{1}_i \otimes 2O_k$, where $\mathbf{1}_i$ is the identity operator on all the spins but the one at site k, and O_k is a generic Hermitian, unitary, and traceless operator [9]. For any translationally invariant and frustration-free Hamiltonian H such that $[H, U_k] \neq 0\ \forall\ U_k$, the vanishing of the EXE is a necessary and sufficient condition for GS factorization [9]. In fact, the minimization defining the EXE identifies an extremal operation $\bar{U}_k$ at each site of the lattice and, therefore, a global operator $\bar{U} \equiv \bigotimes_k \bar{U}_k$ that admits as its own eigenstate the fully factorized state $|G_F\rangle$:

$$|G_F\rangle = \prod_k [\cos(\theta_k/2)|\uparrow_k\rangle + e^{i\varphi_k}\sin(\theta_k/2)|\downarrow_k\rangle], \qquad (2)$$

where θ_k and φ_k define the direction of $\bar{U}_k$ in spin space. $|G_F\rangle$ is the exact GS if and only if the EXE vanishes. Proceeding to investigate frustrated spin models by this method, we consider first the simplest short-range interactions, i.e., antiferromagnetic interactions that extend up to nearest-neighbor (NN) and next-nearest-neighbor (NNN) spins ($r_{\max} = 2$).

Short-range models of frustrated antiferromagnets.— For $r_{\max} = 2$, with ordering $f_1 > f_2 > 0$, in the Hamiltonian Eq. (1) we can set, without loss of generality, $f_1 = 1$, so that the parameter $f = f_2/f_1 \in [0, 1]$ quantifies the degree of frustration: for $f = 0$ the system is frustration free, while for $f = 1$ the model is fully frustrated. To verify the existence of a factorized GS we impose minimization of the energy and the vanishing of the EXE to determine the explicit expressions of θ_k and φ_k. One finds that as long as $f < \frac{1}{2}$ a factorized GS exists and is associated to the single-step antiferromagnetic (SA) order along the x axis. This behavior is mirrored in the fact that $\varphi_k = k\pi$, $\forall\ k$. Vice versa, as soon as $f \geq \frac{1}{2}$, the candidate factorized GS is associated to a dimerized antiferromagnetic order (DA), corresponding to alternating local phases: $\varphi_{2k} = k\pi$, $\varphi_{2k+1} = \varphi_{2k}$ (see Fig. 1). The angle θ_k is site independent: $\theta_k \equiv \theta\ \forall\ k$, and is the solution of

$$\cos\theta = \frac{2h_F}{\mathcal{J}_z - \mathcal{J}_x}, \qquad (3)$$

where h_F stands for the factorizing field, i.e., the value (at this stage, yet to be determined) of the external field at which the GS becomes fully separable. The quantities $\mathcal{J}_\alpha$ are the net interactions that express the coupling of the entire system to a given spin, due to the presence of the external field. The net interaction along the z axis is independent of the magnetic order: $\mathcal{J}_z = 2J_z(1 + f)$, while for the ones along x and y one has $\mathcal{J}_{x,y} = -2(1 - f)J_{x,y}$ in the presence of SA order ($f < \frac{1}{2}$), and $\mathcal{J}_{x,y} = -2fJ_{x,y}$ in the case of DA order ($f \geq \frac{1}{2}$). To prove that the

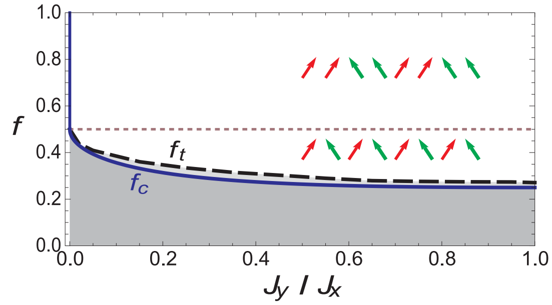

FIG. 1 (color online). Analytical lower bound f_c (solid blue line) and exact numerical value of the frustration compatibility threshold f_t (dashed black line) as functions of the ratio J_y/J_x. GS factorization occurs if and only if $f < f_t$. For f below the horizontal dotted line $f = \frac{1}{2}$ the magnetic order is single-step antiferromagnetic (SA), while for f above it, it is dimerized antiferromagnetic (DA). Therefore, no factorized GS supports DA order, except at $J_y = 0$.

state in Eq. (2) is an eigenstate of the Hamiltonian we decompose the latter at $h = h_F$ into a sum of terms involving only pairs of NN and NNN: $H_{k,k+r} = f_r(J_x S_k^x S_{k+r}^x + J_y S_k^y S_{k+r}^y + J_z S_k^z S_{k+r}^z) - h_f^r(S_k^z + S_{k+r}^z)$, where, consistently with Eq. (3), $h_f^r = f_r \cos\theta[J_z - \cos(\varphi_k) \times \cos(\varphi_{k+r})J_x]/2$. Thus the condition for $|G_F\rangle$ to be an eigenstate of every pair interaction term is

$$-J_y + \cos^2\theta J_x + \cos\varphi_k \cos\varphi_{k+r}\sin^2\theta J_z = 0. \qquad (4)$$

Because Eq. (4) must be satisfied both for the cases in which $\varphi_k = \varphi_{k+r}$ and when $\varphi_k \neq \varphi_{k+r}$, it must be either $\sin\theta = 0$ or $J_z = 0$. The first case ($\sin\theta = 0$) is trivial, as it implies saturation rather than proper factorization. The second possibility ($J_z = 0$) is associated with proper nontrivial factorization, characterized by $\theta \neq 0$. Using Eqs. (3) and (4) one determines exactly the factorizing field:

$$h_F = \frac{1}{2}\sqrt{\mathcal{J}_x\mathcal{J}_y} = \begin{cases} (1-f)\sqrt{J_xJ_y} & f < \frac{1}{2}, \\ f\sqrt{J_xJ_y} & f \geq \frac{1}{2}. \end{cases} \qquad (5)$$

A sufficient condition for $|G_F\rangle$ to be the GS is that its projection over every pair of spins be the GS of the corresponding pair Hamiltonian [10,11]. This condition is never satisfied in the presence of frustration, whose effects cannot be captured by quantities involving only pairs of spins. The method must be generalized to include minimal finite subsets of spins encompassing frustration. In the case of $r_{\max} = 2$, the minimal subset is any block of three contiguous spins, tagged $k - 1$, k, and $k + 1$. The corresponding triplet Hamiltonian term $H_k = \frac{1}{2}H_{k-1,k} + \frac{1}{2}H_{k,k+1} + H_{k-1,k+1}$ includes all the different types of irreducible interactions appearing in the model. Exactly at $h = h_F$ we have that $H = \sum_k H_k$. Moreover, the projection of $|G_F\rangle$ over the Hilbert space of the three spins $k - 1$, k, and $k + 1$ is an eigenstate of H_k. Therefore, if one can show that the projection of $|G_F\rangle$ is the GS of every three-body term H_k, factorization of the total GS is proven. The analysis yields that (i) if $J_y = 0$, the factorized state Eq. (2) is the GS of the systems at $h = h_F$ for all values of the frustration $f \in [0, 1]$, and (ii) if $J_y \neq 0$, the GS is factorized when f lies below a critical value f_c:

$$f_c = \frac{1}{2}\frac{J_x - \sqrt{J_x J_y} + J_y}{J_x + J_y}. \tag{6}$$

To assess whether for $f > f_c$ there may be still a region compatible with GS factorization we consider a partition of the Hamiltonian into blocks of more than three spins. We define the sequence of operators ($\tilde{H}_k^{(n)} = \sum_{\gamma=-n}^{n} H_{k+\gamma}$) which, for any integer n, admit the $(2n+1)$-spin projection of $|G_F\rangle$ as their eigenstate, and whose lowest eigenvalue, in the limit of large n, coincides with the GS energy of the total Hamiltonian H. For every n, the eigenvalue of $\tilde{H}^{(n)}$ associated to the factorized eigenstate is $\varepsilon(n) = (2n-1)\mathcal{E}_F$, where $\mathcal{E}_F$ is the energy density per site at $h = h_F$. Denoting by $\mu(n)$ the minimum eigenvalue of $\tilde{H}^{(n)}$, we have that only if there exists an integer $\bar{n}$ such that $\Delta(n) \equiv \mu(n) - \varepsilon(n)$ vanishes for any $n > \bar{n}$, then the factorized state is associated to the lowest eigenvalues of $\tilde{H}^{(n)}$, and hence it is the GS of the total Hamiltonian H. By studying $\Delta(n)$ as a function of n one can determine exactly, albeit numerically, the actual boundaries separating the occurrence and the absence of GS factorization, as reported in Fig. 1. The exact threshold value f_t lies just slightly above the analytical lower bound f_c, Eq. (6).

Summarizing, we have shown that for $f < f_t$, short-range frustrated models admit an exact, separable GS of the form Eq. (2) when the external magnetic field h takes the value h_F defined by Eq. (5). The associated magnetic order is SA, while every factorized state associated to a DA order is always an excited energy eigenstate; it becomes a GS only exactly at $J_y = 0$. Because the existence of factorized energy eigenstates is always associated to a violation of the parity symmetry of the magnetization along the direction of the external field [10,11] the proof of the existence of factorized GSs, even if it yields no direct information on the location of the quantum critical points h_c, warrants the existence of quantum phase transitions to an ordered phase, in frustrated models, as the external field h decreases and crosses h_c (in the case that we have illustrated, it is a transition to a SA order along x). Moreover, since the factorizing field h_F necessarily lies in the ordered region, one can, at least, conclude that the factorizing field anticipates the critical one from below: $h_F \leq h_c$, a behavior already evidenced in some frustration-free models [12]. Exactly at $f = f_t$ the system undergoes a level crossing, and hence a first order phase transition from the twofold degenerate factorized GS Eq. (2) to a twofold degenerate entangled GS state with complex long range order (spin liquid phase) incompatible with factorization points. This phenomenon identifies a frustration-driven entangling-disentangling transition of the GS at $h = h_F$ as f crosses the critical threshold f_t dividing the regimes of weak and strong frustration.

A phenomenological measure of frustration in antiferromagnetic models is provided by T_{CW}/T_N, i.e., the ratio of the Curie-Weiss temperature to the Néel temperature of bulk three-dimensional ordering [13]. This definition cannot be applied to systems with vanishing T_N (like, e.g., 1D and 2D models) and it cannot distinguish between different contributions, classical and quantum, to frustration. Notwithstanding these limitations, our ground-state analysis suggests that this phenomenological measure does capture some aspects of frustration, as follows. The existence of a factorized GS implies the existence of a transition to an ordered phase, as we argued above. In a bulk 3D system this should correspond to a finite value of the ratio T_{CW}/T_N, since the order would necessarily freeze at a finite value of $T_N > 0$. On the other hand, in strongly frustrated models, strong correlations between quantum fluctuations persist in the presence of an applied field favoring GS factorization, and the existence of ordered phases tends to be suppressed. In the corresponding bulk 3D systems one should then find a higher, asymptotically diverging value of the ratio T_{CW}/T_N, as the temperature at which the order freezes approaches the absolute zero.

Models with interactions of arbitrary finite range.—For models Eq. (1) with finite $r_{\max} > 2$ the triplet Hamiltonians H_k are generalized to subsets of $r_{\max} + 1$ spins, with constraint $\sum_k H_k = H$ at $h = h_F$. The space of the Hamiltonian parameters is still divided in a region of low frustration compatible with GS factorization, and one of high frustration for which GS factorization is forbidden, as shown in Fig. 2 for models with maximum range of interaction $r_{\max} = 4$ that include, for instance, the $J_1 - J_2 - J_3 - J_4$ and $J_1 - J_2 - J_3$ models. Two general trends are observed: for $J_y \neq 0$, the factorized GS has SA order along the x axis and, as shown in Fig. 1 and 2, the region of low frustration allowing GS factorization decreases as the anisotropy J_y/J_x increases.

Models with interactions of infinite range.—If in Eq. (1) we let $f_r \to 0$ when the maximum interaction range $r_{\max} \to \infty$, the question of the existence of factorized energy eigenstates can be analyzed by neglecting all the

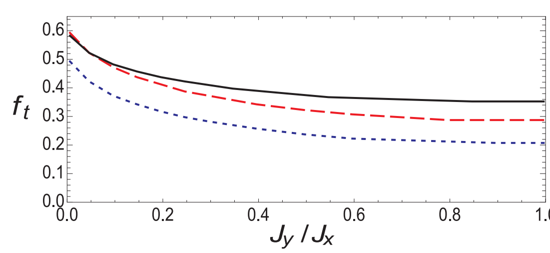

FIG. 2 (color online). Threshold value of the frustration, f_t, below which GS factorization occurs, for frustrated antiferromagnets with $r_{\max} = 4$, as a function of J_y/J_x. Solid black line: $f_2 = f$; $f_3 = f^2$; $f_4 = f^3$. Dashed red line: $f_2 = f$; $f_3 = f/2$; $f_4 = f/3$. Dotted blue line: $f_2 = f$; $f_3 = f/2$; $f_4 = f/4$.

interactions between spins at distances greater then some cutoff value r', solve the associated constraints, and then let $r' \to \infty$. To this aim, for each r' we consider the operator $H_k^{(r')} = \frac{1}{2}\sum_{\gamma=-r'}^{r'}\sum_{\gamma'=-r'}^{r'}(1-\delta_{\gamma-\gamma'}) \times \frac{1}{2r'+1-|\gamma-\gamma'|}H_{\gamma,\gamma'}$ that expresses the sum of all the pair interaction terms between the r' spins closest to k, and the associated quantity $\Delta(r') = \mu(r') + \frac{1}{4}(J_x + J_y) \times \sum_{k=1}^{r'}(-1)^k f_k$, where $\mu(r')$ is the lowest eigenvalue of $H_k^{(r')}$. We have then analyzed different decay laws for f_r, i.e., fast, $f_r = 1/r^2$, intermediate, $f_r = 1/r$, and slow, $f_r = 1/\sqrt{r}$. In the first case it is always $\Delta(r') = 0$ and consequently the system admits a factorized GS exactly at $h_F = (\pi^2/12)\sqrt{J_x J_y}$. In the second case ($f_r = 1/r$), according to the numerical evidence, $\Delta(r')$ vanishes in the limit of arbitrarily large r' and GS factorization appears to occur at $h_F = \ln(2)\sqrt{J_x J_y}$. Finally, in the case of slow decay ($f_r = 1/\sqrt{r}$), one has that $\Delta(r') \neq 0\ \forall\ r'$ and therefore no factorized GS can exist. Therefore, fully connected models characterized by a rapidly decaying f_r, and hence by low frustration, allow for GS factorization and the associated SA or DA orders. Vice versa, models with slowly decaying f_r, corresponding to strong frustration, do not admit factorized GS and simple mean-field and classical-like descriptions.

Frustrated quantum models of complex condensed matter and biological systems.—The ANNNI (axial next-nearest-neighbor Ising) model, a particular case of the general class of models that we consider in the present work, provides a possible effective description of systems with long-period modulated structures, such as, e.g., polytypism, antiphase boundaries in binary alloys, and helical phases in rare earths compounds [4]. It is thought that quantum frustration effects may be the mechanism responsible for the observed stability of these structures, and for this reason the quantum version of the ANNNI model is being intensively studied [4]. It is then important to establish whether stable modulated structures are indeed predicted at all by the quantum ANNNI model and in what physical regimes. When applied to the quantum ANNNI model ($J_y = J_z = 0$), our analysis proves that the mean-field description is applicable for all values of the frustration and that the value $f = \frac{1}{2}$ discriminates between two types of stable structures, a simple unmodulated ferromagnetic order associated to a fully factorized GS for $f < \frac{1}{2}$ and an antiphase modulated GS with DA order for $f > \frac{1}{2}$.

Models of frustrated quantum spin networks have also been advocated as effective descriptions of gene expression and complex genomic patterns [5]. Here, again, the problem arises of the range of applicability of simple mean-field descriptions corresponding to simple magnetic orders. Indeed, much as for neural networks, the landscape of stable attractors in gene networks depends, classically, on the degree of frustration. Assuming a description based on frustrated classical models with long-range interactions leads to the qualitative prediction of a small number of stable attractors in the presence of a "sufficiently" weak frustration. The question is then whether this prediction is stable against the effects of quantum fluctuations. Our analysis shows that the mean-field picture is qualitatively correct and makes it quantitative by determining the boundary between the weak and the strong frustration regime, in which the mean-field predictions fail. For models with long-range interactions, as we have shown above (see Fig. 2), the region of low frustration consistent with a mean-field description is determined by the anisotropy ratio J_y/J_x and decreases as the latter is increased.

Conclusions and outlook.—We have introduced a rigorous criterion for discriminating between weakly and strongly frustrated quantum systems in terms of GS factorizability. We have determined the threshold that separates the regions of weak and strong frustration, and we have singled out the exact forms of the factorized GS, the associated quantum phases, and the corresponding magnetic orders in the region of low frustration. These criteria should be experimentally testable in two- and three-body correlation experiments.

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