

Separability and ground-state factorization in quantum spin systems

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We investigate the existence and the properties of fully separable (fully factorized) ground states in quantum spin systems. Exploiting techniques of quantum information and entanglement theory, we extend a recently introduced method and construct a general, self-contained theory of ground state factorization in frustration-free quantum spin models defined on lattices in any spatial dimension and for interactions of arbitrary range. We show that, quite generally, nonexactly solvable translationally invariant models in presence of an external uniform magnetic field can admit exact, fully factorized ground state solutions. Unentangled ground states occur at finite values of the Hamiltonian parameters satisfying well-defined balancing conditions between the applied field and the interaction strengths. These conditions are analytically determined together with the type of magnetic orderings compatible with factorization and the corresponding values of the fundamental observables such as energy and magnetization. The method is applied to a series of examples of increasing complexity, including translationally invariant models with short, long, and infinite ranges of interaction, as well as systems with spatial anisotropies, in lower and higher dimensions. We also illustrate how the general method, besides yielding a large series of exact results for complex models in any dimension, recovers, as particular cases, the results previously achieved on simple models in low dimensions exploiting direct methods based on factorized mean-field ansatz.

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I. INTRODUCTION

Quantum information theory is an area of scientific investigation that has witnessed an enormous progress in the last decade.¹ In the framework of quantum information science, paradigmatic systems of condensed matter physics such as, e.g., spin chains and harmonic lattices are analyzed from the point of view of their information content and ability to process and transfer information. Fundamental concepts of statistical mechanics and probability, such as the Shannon-von Neumann entropy,² play a central role in the quantification of bipartite quantum entanglement.³ On the other hand, exciting advances in quantum information research are in a sense paying back the debt: the mathematical and theoretical toolkits developed for the characterization and quantification of quantum entanglement have proven useful to tackle questions and improve our understanding in the investigation of strongly correlated systems and quantum phase transitions.⁴

Perhaps the most interesting development stemming from the application of the tools of entanglement theory concerns the study of correlation scaling in diversely connected systems, with its relations to conformal field theory and the proof of longstanding conjectures on entropic area laws in spin and harmonic lattice systems.⁵ These investigations and the associated results are of fundamental interest because they allow to enhance the control and establish firmer bounds and limits of applicability on many important tools of simulation and numerical analysis of complex many-body systems, a fundamental task in condensed matter, such as the density-matrix renormalization group algorithms,⁶ matrix product representations,⁷ the entanglement renormalization ansatz,⁸ and weighted graph states methods.⁹

The pioneering application of quantum information concepts to the condensed matter was the observation that two-body entanglement, as quantified by the concurrence, in the ground state of a cooperative system, exhibits peculiar scaling features approaching a quantum critical point.¹⁰ These seminal studies helped to clarify that at quantum phase transitions,¹¹ the dramatic change in the ground state of a many-body system is associated to, or reflected by, a change in the way that quantum fluctuations are correlated, i.e., in the way entanglement is distributed among the elementary constituents. Many recent efforts have thus been aimed at understanding the behavior of different measures of entanglement at quantum phase transitions and assessing the corresponding enhancement of properties useful for applications in quantum technology and quantum engineering.⁴ However, since most entanglement measures can be often rewritten in terms of the conventional n -point correlation functions, the presence of a divergence in the former at quantum criticality can be directly traced back to a divergence in the latter,¹² although in some particular instances entanglement-based studies allowed to discover different types of phase transitions.¹³

Finally, a more technologically oriented product of the interaction between these two areas of research is the study of quantum spin chains as natural information carriers and distributors,¹⁴ able to realize tasks such as quantum state transfer¹⁵ and storage,¹⁶ possibly with maximal fidelity in chains with suitably engineered couplings and dynamics.

Quantum engineering and quantum technology are being indeed developed at a fast pace. Quantum devices are vigorously pursued for applications ranging from nanosciences to quantum computation and entanglement-enhanced

metrology.¹⁷ Despite a large variety of possible implementations involving different physical systems, many relevant properties of such devices can be, in fact, investigated in a unified setting by appropriate mappings to quantum spin models.^{18,19} Control of separability and entanglement in ground states of quantum spin models plays an important role in entanglement-enabled quantum technology applications and needs to be characterized and quantified in different physical regimes.⁴ From a more fundamental perspective, the determination of exact solutions endowed with precisely known properties of separability or entanglement, can be of great relevance in the study of advanced models of condensed matter and cooperative systems that are, in general, not exactly solvable.

In this paper we exploit quantum information tools to tackle another important problem in condensed matter physics: the determination and characterization of exact ground states of cooperative systems characterized by the property of being in the form of a fully factorized tensor product of single-particle pure states, with no quantum correlations between the individual constituents. Historically, the occurrence of totally factorized (unentangled) ground states of quantum many-body systems was first discovered in the one-dimensional (1D) anisotropic Heisenberg model with nearest-neighbor interactions by Kurmann *et al.*,²⁰ by adopting a direct method in terms of product state ansatz. This result was later rederived and extended to two dimensions using quantum Monte Carlo numerical methods.²¹ The direct product-state ansatz method of Kurmann *et al.* has been later extended to anisotropic rings with interactions of arbitrary range, by exploiting the observation that factorized ground states break the parity symmetry.^{22,23} Complex quantum systems exhibiting cooperative behaviors, whose ground states are typically entangled,²⁴ may thus admit, for some nontrivial values of the Hamiltonian parameters, a ground state which is completely separable. The occurrence of factorization at finite or even strong values of the couplings is thus an effect of a delicate balancing between interactions and external fields.

The phenomenon of ground state factorization is particularly intriguing as it appears to be associated with the presence of an “entanglement phase transition” with no classical counterpart.²⁵ Furthermore, for the purposes of quantum engineering applications, that employ distributed entanglement in order to manipulate and transfer information,¹⁴ factorization points need to be exactly identified and either avoided, in order to guarantee the reliable implementation of quantum devices, or properly exploited for the dynamical creation of strongly entangled multipartite states of large assemblies of microsystems (graph and cluster states). Finally, and also quite importantly, for models not admitting exact general solutions, achieving knowledge of the exact ground state, even if only for the restricted nontrivial set of parameters associated to factorization, would allow (i) to prove the existence of an ordered phase and characterize it and (ii) to build variational or perturbative approximation schemes around the exact factorized solution, that may then be used as test benchmarks for the validity and the precision of numerical algorithms and simulations. Unfortunately, the direct method based on the ansatz of a factorized solution is neither suffi-

ciently general nor mathematically tractable, apart from the notable exceptions of one-dimensional spin chains with short-range,²⁰ infinite-range,²⁶ and some types of long-range exchange interactions.^{22,23}

In a recent work²⁷ we introduced an analytic method that allows to determine exactly the existence of factorized ground states and to characterize their properties in quantum spin models defined on regular lattices of any size (finite as well as at the thermodynamic limit), in any spatial dimension, and with spin-spin interactions of arbitrary range. In correspondence to rigorously established ground state factorizability, the method also allows to determine sets of exact solutions in generally nonexactly solvable models. All the previous particular findings can be rigorously rederived and extended within a unified framework inspired by concepts of quantum information science.

In the present work we extend the original method introduced in Ref. 27 and we develop a general self-contained theory of ground state factorization in (frustration-free) quantum spin systems: with no *a priori* assumption on the nature of the magnetic ordering, we derive a complete and closed set of conditions that have to be satisfied by the Hamiltonian interaction parameters in order for the ground state to be factorized, at precisely determined values of the external magnetic field, with well-defined values of the magnetization and of the energy. Besides the completely rigorous rederivation of the few previously known results on quantum factorization points,^{20–23,26} our general analytic method allows to determine exact factorization points and factorized ground states in, generally nonexactly solvable, spin-1/2 models as well as in the corresponding Hamiltonian models of any higher spin. These results hold true regardless of spatial dimensionality and interaction range, and can be easily extended even to nontranslationally invariant systems. We illustrate the versatility of the method with a series of different applications, including models with nearest-neighbor interactions (for which we provide the full factorization diagram, generalizing the results of Refs. 20, 22, and 23, and of our recent work²⁷), models with long-range interactions (notably including, among others, the fully connected infinite-range Lipkin-Meshkov-Glick (LMG) model²⁶ and systems with unbalanced next-to-nearest-neighbor interactions on cubic lattices), and models with spatial anisotropies.

The paper is organized as follows. An excursus on the problem of ground state factorization is presented in Sec. II. In Sec. III we recall the quantum information toolkit upon which our method is based on, in particular the formalism of single-spin or single-qubit, unitary operations, and associated entanglement excitation energies, previously introduced for the characterization and quantification of bipartite entanglement from an abstract geometrical perspective.^{28,29} The general method for the rigorous determination of factorized ground states, that generalizes the scheme introduced in Ref. 27, is discussed in full detail in Sec. IV. Relevant applications and examples, including models defined on lattices of different spatial dimensions and with different interaction ranges as well as extensions to models with spatial anisotropies and with dimerized interactions are discussed in Secs. V–VIII. Concluding remarks and outlooks on future perspectives are presented in Sec. IX.

II. THEORY OF GROUND STATE FACTORIZATION: STATE OF THE ART

Quantum fluctuations in the ground states of cooperative many-body systems are typically highly correlated, i.e., those states contain in the most general instance a strong degree of entanglement distributed among the individual components. This is one of the reasons why their exact characterization is often hard to be accomplished by analytical or even numerical methods. However, there may exist particular solutions corresponding to special values of the Hamiltonian parameters such that the ground state becomes “classical-like,” in the sense of being a full product state of single-site factors (completely separable, fully factorized state). It is quite surprising that despite the inherent appeal of such exact, special solutions, and the renewed interest stemming from possible applications to quantum technology, very few analytical advances were obtained in the last quarter of a century.

A. Direct method: Product state ansatz

The first systematic work on ground state factorization in quantum spin models was completed by Kurmann *et al.*²⁰ in 1982. They focused on the one-dimensional nearest-neighbor anisotropic Heisenberg-type antiferromagnetic spin-1/2 model in transverse field, with the assumption that all the spin-spin couplings take non-negative values. Kurmann *et al.* identified a precise value of the external magnetic field, the “factorizing field,” corresponding to which the system admits a fully factorized ground state. They employed a very direct, “brute force” method, i.e., formulating a product state ansatz and verifying if and for what values of the Hamiltonian parameters it satisfies the stationary Schrödinger problem with lowest energy. Even though this approach appears obvious and extremely easy to pursue, the positive result obtained by Kurmann *et al.* in the case of the 1D Heisenberg model was enabled by some special properties of the case they analyzed. In fact, in order to verify the eigenvalue equation for the product state ansatz, one needs to decompose the total Hamiltonian of the system into a series of pairwise terms, which could be done easily for the model studied by Kurmann *et al.* since all the “pairwise components” of the factorizing magnetic field had the same weight in this particular case. However, this direct method of determining factorization is in fact significantly less obvious, useful, and comprehensive, when one tries to apply it to more general cases. For instance, considering models with interaction terms of growing spatial range, and/or increasing the spatial dimensionality of the lattice, and/or treating extensions to spatially anisotropic or nontranslationally invariant models, results in increasingly hard “guesses” concerning the partitioning of the external field into pairwise components and in increasingly nontrivial verification steps. Depending on the structure of the model and on the form of the product state ansatz, the direct method may either fail to detect factorization points at all, or it may detect only a subset of all physically realizable factorized solutions, or finally it may lead to intractable sets of conditions. These limitations of the direct method become evident, as we will see in the following, even in the simplest 1D XYZ model with nearest-neighbor

interactions analyzed by Kurmann and co-workers. In their original work, due to the insufficient generality of their proposed product ansatz, they failed to identify a wide range of situations that allow the existence of factorized ground states. As we will see when discussing models with competing interactions of different spatial ranges, a further serious fault of the direct method, that becomes incurable in the presence of frustration, is its incorrect assessment of factorized ground states that are in fact excited energy eigenstates of the system.

Following the seminal analysis by Kurmann *et al.*, the direct method has been applied to the fully connected infinite-range Lipkin-Meshkov-Glick model by Dusuel and Vidal,²⁶ and to the anisotropic Heisenberg chain with the same interactions of arbitrary range along the three spatial directions by Hoeger *et al.*²² and by Rossignoli *et al.*²³ We would like to remark that these works, that include the results of Refs. 20 and 26 as special cases, provide an interesting characterization of factorization points in finite (one-dimensional) translationally invariant lattice spin models with periodic boundary conditions as those points where the parity symmetry is broken.

B. Quantum informatic approach

A general and rigorous approach to the problem of ground state separability, completely different from the direct method based on the product state ansatz, has been introduced by us in Ref. 27 and is fully developed in the present work. This analytic method allows *inter alia* to complete the factorization diagram of the anisotropic spin-1/2 models without restrictions on the sign of the couplings, and to go significantly beyond the limitations of the previously mentioned studies. Our approach is based on an additional characterization of product states (including product ground states) that employs concepts and tools of quantum information and entanglement theory. The strong point of the quantum informatic approach to ground state factorization lies in its generality and its ensuing independence from the types and ranges of interactions present in the Hamiltonian, the lattice size, and the spatial dimension, which makes it applicable in the most general cases and therefore especially useful in all the situations that are either intractable or incomplete if one resorts to the direct method or to numerical techniques.

In fact, in the original formulation of the quantum informatic method²⁷ there was still trace of a residual “ansatz” in the initial stage, since the magnetic ordering of the candidate factorized ground state had to be in some sense guessed, and imposed *a priori*. Moreover, in the final stage, we were not yet able to derive a completely general set of conditions in order to determine in each situation whether a candidate factorized state that turned out to belong to the spectrum of the Hamiltonian was actually a ground state or belonged to the set of excited states. This had then to be decided case by case in each specific instance.

In the present work we proceed further and develop the complete method to determine and characterize factorized ground states in quantum cooperative systems. We provide

the systematics that allows to determine the occurrence of full ground state separability given a generic quantum spin Hamiltonian. The magnetic ordering is derived as a consequence of the theory and not imposed *a priori*. A complete set of general conditions is established for the verification of ground state factorization, and the elegance of the method does not hinder practical usefulness in the application to specific models and situations.

We would like to recall that numerical advances on the problem of ground state factorization have been realized by the Monte Carlo study of ground state factorization in two-dimensional anisotropic nearest-neighbor spin models.²¹ Unfortunately, beyond this important result the numerical approach appears to have a very restricted potential for extensions, since the required computational power increases rapidly with the spatial dimension and/or with the range of interactions. We will show that the difficulties inherent to the direct analytic approach and to the numerical method are intrinsically absent in our formalism.

III. SINGLE QUBIT UNITARY OPERATIONS AND ENTANGLEMENT EXCITATION ENERGIES

In this section we provide a brief overview of some recent results on the geometrical interpretation of the entanglement measure known as “tangle” (linear entropy)²⁸ and the consequences it entails for the relationship between energy and pairwise entanglement.²⁹ Such results embody the premises for our all-analytic characterization of ground state separability in quantum spin systems.

Here and in the following we consider generic systems made of N spin-1/2 elementary constituents, or, in the language of quantum information, N qubits. For such a system, we introduce the set of single-qubit unitary operations (SQUOs) U_k ,²⁸ defined as the unitary transformations that act separately as the identity on any spin of the system except the k th one, on which they act instead as Hermitian, unitary, and traceless operators:

$$U_k \equiv \bigotimes_{i \neq k} 1_i \otimes 2O_k. \quad (1)$$

In Eq. (1) 1_i stands for the identity operator on the i th spin of the system while the generic Hermitian, unitary, and traceless operator O_k can be expressed as a linear combination of the standard spin operators (S_k^α) defined on the k th spin

$$O_k = \sin \theta_k \cos \varphi_k S_k^x + \sin \theta_k \sin \varphi_k S_k^y + \cos \theta_k S_k^z. \quad (2)$$

In the previous definition the parameters θ_k and φ_k take values, respectively, in the ranges $(-\pi/2, \pi/2]$ and $[0, 2\pi)$. Physically, O_k corresponds to a rotation in the spin space, and the traceless condition imposes the rotation operation to be orthogonal to the identity, so basically a combination of spin flip and phase flip.

A SQUO transforms every pure state $|\Psi\rangle \in \mathbb{C}^{2N}$ into a new state $|\tilde{\Psi}\rangle = U_k |\Psi\rangle$, that in general differs from $|\Psi\rangle$. We may quantify the action of the SQUO in terms of the trace distance between the original and the transformed state, defined as $D(U_k; |\Psi\rangle) = D(\theta_k; \varphi_k; |\Psi\rangle) \equiv \sqrt{1 - |\langle \Psi | U_k | \Psi \rangle|^2}$. The distance D varies in the interval $[0, 1]$ and vanishes if and only if

the two states coincide, meaning that the considered SQUO leaves the original state unchanged. For a given initial state and for any site k , one can determine the *Extremal*-SQUO (E-SQUO) that minimizes such a distance. One can prove that the E-SQUO is uniquely determined by the following conditions on the angular variables:²⁸

$$\begin{aligned} \bar{\varphi}_k &= \arctan \left(\frac{\langle S_k^y \rangle}{\langle S_k^x \rangle} \right), \\ \bar{\theta}_k &= \arctan \left(\frac{\langle S_k^x \rangle \cos \bar{\varphi} + \langle S_k^y \rangle \sin \bar{\varphi}}{\langle S_k^z \rangle} \right), \end{aligned} \quad (3)$$

where $\langle S_k^\alpha \rangle$ denotes the expectation value of the spin operator S_k^α on the unperturbed state $|\Psi\rangle$ ($\langle S_k^\alpha \rangle = \langle \Psi | S_k^\alpha | \Psi \rangle$). The E-SQUO plays a crucial role in our analysis: For any pure state defined on a general system of interacting qubits one can prove²⁸ that the square of the distance associated to the action of the E-SQUO coincides with the linear entropy $S_L(\rho_k) = 1 - \text{Tr}[\rho_k^2]$ of the k th qubit (where ρ_k denotes the reduced density matrix of qubit k). This quantity, also known as the *tangle* τ in the literature, is an entanglement monotone for qubit systems and satisfies important monogamy constraints.³⁰ Being a monotonic function of the von Neumann entropy of entanglement,³¹ it quantifies the bipartite block entanglement present in the state $|\Psi\rangle$ between spin k and the remaining $N-1$ constituents, and is thus a proper measure of single-site entanglement.³² One has the following relation:²⁸

$$\begin{aligned} D^2(\bar{U}_k; |\Psi\rangle) &= \tau_{k|\forall j \neq k}(|\Psi\rangle) \equiv 4 \text{Det} \rho_k \\ &= 1 - 4[\langle S_k^x \rangle^2 + \langle S_k^y \rangle^2 + \langle S_k^z \rangle^2]. \end{aligned} \quad (4)$$

This geometric-operational characterization of the tangle allows to develop a quantum informatic approach to the problem of characterizing the correlation properties of the ground state in many-body quantum systems.²⁹ Let us consider a collection of spin-1/2 systems defined on a regular lattice, with Hamiltonian H , and let $|\Psi\rangle$ denote from now on the ground state of H . If the system is in the ground state, the application of a SQUO on a generic spin of the lattice is necessarily associated to an energy transfer that one must provide to the system in order to realize the selected SQUO. In other words, a SQUO perturbs the system, and this perturbation results in an increase in the average energy (obviously, in general the transformed state needs not to be an eigenstate of the Hamiltonian). Such energy deviation from the ground state value can be quantitatively defined as

$$\Delta E(U_k) \equiv \Delta E(\theta_k, \varphi_k) = \langle \Psi | U_k^\dagger H U_k | \Psi \rangle - \langle \Psi | H | \Psi \rangle. \quad (5)$$

Because $|\Psi\rangle$ is the ground state of H , $\Delta E(U_k)$ is a non-negative defined quantity. Considering the special relation between the E-SQUO and the tangle we may expect that the associated amount of energy difference $\Delta E(\bar{U}_k)$, appropriately named “entanglement excitation energy” (EXE), will have as well a strong, direct connection with the tangle and in general with the single-site entanglement in the ground state. In fact, starting from the above definition of Eq. (5) and taking into account the property of the E-SQUO of leav-

ing unchanged a fully disentangled state, it has been established in full generality²⁹ that if the system is invariant under spatial translation and the Hamiltonian of the system does not commute with any possible SQUO, then the vanishing of the EXE is a *necessary and sufficient* condition to admit a fully factorized ground state $|\Psi\rangle$.²⁹ Hence, if the system that we want to analyze satisfies all the former hypotheses, the vanishing of the EXE provides an additional condition, besides the vanishing of the tangle τ , that one needs to include in establishing a general analytic approach to the problem of ground state factorization.

IV. THEORY OF GROUND STATE FACTORIZATION: GENERAL ANALYTIC METHOD

A. Preliminaries

The general method that was first partially developed in Ref. 27 for the determination of existence, location, and exact form of factorized ground states rests on the following two main observations: (i) the ground state $|\Psi\rangle$ of a spin-1/2 Hamiltonian H is factorized if and only if the single-site entanglement (tangle) τ vanishes for all spins k in the lattice; (ii) provided that $[H, U_k] \neq 0$ for every possible SQUO U_k of the form Eq. (1), the ground state $|\Psi\rangle$ of a spin-1/2 Hamiltonian H is factorized if and only if the EXE $\Delta E(\bar{U}_k) = \langle \Psi | \bar{U}_k H \bar{U}_k | \Psi \rangle - \langle \Psi | H | \Psi \rangle$ vanishes $\forall k$.

In Ref. 27, the strategy to the determination and understanding of factorization for a given Hamiltonian bore on the above two facts and on the requirement to assume as working point a phase endowed with some kind of magnetic order. By imposing the vanishing of the EXE and of the tangle, we showed how to determine uniquely the form of the completely disentangled state compatible with the assumed magnetic order, candidate to be the ground state of the system at a particular value of the external magnetic field (labeled as “factorizing field”). The final steps of the procedure concern the determination of exact analytic conditions for the candidate factorized state to be an eigenstate of the Hamiltonian with lowest energy. In Ref. 27, we derived a closed set of eigenstate conditions, but establishing whether a factorized eigenstate is actually a ground state had to be left to a case by case analysis.

In the present paper we generalize the method, extend its scope, and apply it to different classes of quantum spin models. First, we will show that there is no need for *a priori* assumptions on the magnetic order. In fact, we will prove that the existence of a factorized ground state is a necessary and sufficient condition for the existence of quantum phase transitions and ordered phases in translationally invariant quantum spin models with exchange interactions and in the presence of external fields. Moreover, the actual structure of the factorized ground state determines automatically the kind of ordered phase. Further, we derive a complete set of rigorous conditions for the candidate disentangled state to be an eigenstate and a ground state. In particular, for systems with no frustration we prove that if the factorized state is an eigenstate, then it is always a ground state of the system.

B. Quantum spin models on regular lattices

We illustrate the method in detail by considering its application to the general, translationally invariant, exchange

Hamiltonian H for spin-1/2 systems on a D -dimensional regular lattices, with spin-spin interactions of arbitrary range and arbitrary anisotropic couplings

$$H = \frac{1}{2} \sum_{\underline{i}, \underline{l}} J_{\alpha}^r S_{\underline{i}}^{\alpha} S_{\underline{l}}^{\alpha} + J_z^r S_{\underline{i}}^z S_{\underline{l}}^z - h \sum_{\underline{i}} S_{\underline{i}}^z. \quad (6)$$

Here \underline{i} (and similarly \underline{l}) is a D -dimensional index vector identifying a site in the lattice, $S_{\underline{i}}^{\alpha}$ ($\alpha=x, y, z$) stands for the spin-1/2 operator on site \underline{i} , h is external field directed along the z direction, $r=|\underline{i}-\underline{l}|$ is the distance between two lattice sites, and J_{α}^r is the spin-spin coupling along the α direction. Translational invariance is ensured by the fact that all the couplings depend only on the distance r between the spins. This type of Hamiltonian encompasses a large variety of models and spans over several universality classes including, among others, the Ising, XY, Heisenberg, and XYZ symmetry classes. Besides their importance in quantum statistical mechanics and in the theory of quantum critical phenomena, these models play an important role in the study of various schemes of quantum information and quantum communication tasks with quantum many-body systems.¹⁴

It is a rather straightforward exercise to verify that the Hamiltonian (6) never commutes with the SQUOs $U_k \forall k$. Translational invariance and noncommutativity of the Hamiltonian with the SQUOs guarantee that the vanishing of the EXE is a necessary and sufficient condition for the full separability of the ground state [statement (ii) above]. Since the external field h is uniform on the lattice, it forces the existence of a site-independent, nonvanishing magnetization M_z along the z axis: $\langle S_k^z \rangle \equiv M_z \forall k$. On the other hand, at a factorization point, statement (i) above imposes the vanishing of the single-site entanglement on all sites of the lattice. Therefore, if a factorization point exists, the magnetizations along the directions orthogonal to the external field must assume the following form:

$$\begin{aligned} \langle S_k^x \rangle &\equiv M_k^x = M_{\perp} \cos \varphi_k, \\ \langle S_k^y \rangle &\equiv M_k^y = M_{\perp} \sin \varphi_k, \end{aligned} \quad (7)$$

where $M_{\perp} = \sqrt{\frac{1}{4} - M_z^2}$ is the modulus of the projection of the magnetization on the xy plane and the local orientations φ_k , and hence the type of magnetic ordering in the xy plane, remain undetermined. Since M_z is site independent, then M_{\perp} is site independent as well. Taking into account Eq. (3) of Sec. III one sees that, at least at the factorization point, $\bar{\theta}_k$, i.e., one of the two angles that fix the orientation of the E-SQUO, does not depend on the site index. Therefore $\bar{\theta}_k \equiv \theta \forall k$.

Collecting the former results and considering that in the presence of a factorized ground state, if it exists, all the correlation functions are products of single-site expectations values, we obtain that the condition on the vanishing of the EXE associated to the generic site k reads

$$\begin{aligned} \frac{\Delta E(\bar{U}_k)}{2} = 0 = & -\sin \theta (\sin \theta M_z - \cos \theta M_\perp) \left(M_z \sum_i J_{k,i}^z - h_f \right) \\ & + \cos \theta M_\perp (\sin \theta M_z - \cos \theta M_\perp) \\ & \times \left(\cos \varphi_k \sum_i J_{k,i}^x \cos \varphi_i + \sin \varphi_k \sum_i J_{k,i}^y \sin \varphi_i \right). \end{aligned} \quad (8)$$

In the former equation h_f is the *factorizing field*, i.e., the value, if it exists, of the external field for which ground state factorization occurs.

Since we are looking for a fully factorized ground state, Eq. (8) must be satisfied simultaneously for all k and, henceforth, Eq. (8) must be site independent. This fact in turn implies that the following relation must be satisfied by every angle φ_k

$$\cos \varphi_k \sum_j J_x^r \cos \varphi_j + \sin \varphi_k \sum_j J_y^r \sin \varphi_j = K. \quad (9)$$

Equation (8) must hold independently of the site in which the E-SQUO acts and the value of the constant K must be identified by determining the expression of the energy density, i.e., the energy per site, associated to the factorized ground state. Given the total ground state energy E and the total number of sites N , the latter quantity can be written as

$$\begin{aligned} \frac{E}{N} = & \frac{1}{2} M_z^2 \sum_r Z_r J_z^r - h_f M_z + \frac{1}{2} M_\perp^2 \sum_j J_x^r \cos \varphi_k \cos \varphi_j \\ & + J_y^r \sin \varphi_k \sin \varphi_j \\ \equiv & \frac{1}{2} M_z^2 \sum_r Z_r J_z^r - h_f M_z + \frac{1}{2} M_\perp^2 K, \end{aligned} \quad (10)$$

where Z_r is the coordination number, that is the number of sites at distance r from a given site. In order to determine the magnetic order in the candidate factorized ground state, one can now exploit the fact that, by definition, it must minimize the energy of the system. Therefore such state will be simply characterized by the magnetic order that minimizes the per site contribution K , depending on the Hamiltonian parameters and the geometric structure of the lattice. Thus the general conditions for full separability of the ground state lead to the uncovering of the magnetic order in the xy plane. In the original formulation of the quantum informatic method²⁷ one had to assume from the beginning the type of ordered phase, and this resulted in constraints on the magnetization and limitations in the range of the coupling coefficients.

C. Magnetic orders and factorization

The outcome of the minimization of the energy density depends on the presence or the absence of frustration in the system, either due to the lattice geometry, or to the structure of the Hamiltonian, or to both causes. For Hamiltonians belonging to the class of Eq. (6), frustration can be due both to the geometry of the lattice, e.g., for systems with nearest-neighbor antiferromagnetic interactions defined on a lattice that admits closed loops with an odd number of spins, and to

the competition of interactions of different spatial orders, e.g., in systems defined on linear chains with nearest-neighbor ferromagnetic and next-nearest-neighbor antiferromagnetic interactions. Frustration effects in systems with interactions of different spatial ranges arise whenever it happens that the minimization of the energy associated to interactions over a certain spatial scale precludes the possibility of minimizing the energy associated to interactions over a different spatial scale. In the absence of frustration, i.e., when the lattice geometry and the interactions between the spins are such to allow all energy minimizations simultaneously, it is straightforward to prove that every possible factorized ground state must be characterized by one of only four magnetic orders out of the many possible ones. The complete proof of this statement is reported in Appendix. This restricted set includes ferromagnetic ordering along the x direction ($\varphi_k=0 \forall k$) or along the y direction ($\varphi_k = \pi/2 \forall k$), and antiferromagnetic ordering along the x direction ($\varphi_k=|k|\pi \forall k$) or along the y direction ($\varphi_k=(\pi/2) + |k|\pi \forall k$). By requiring the minimization of the energy per site, Eq. (10), the type of order effectively present in the ground state can be determined by comparing the values of the different “net interactions” along the x and y directions, where the net interactions are defined as follows:

$$\begin{aligned} \mathcal{J}_\alpha^A = & \sum_{r=1}^{\infty} (-1)^r Z_r J_\alpha^r; \\ \mathcal{J}_\alpha^F = & \sum_{r=1}^{\infty} Z_r J_\alpha^r, \end{aligned} \quad (11)$$

with $\alpha=x,y$. The net interaction along the z direction is defined equivalently as

$$\mathcal{J}_z^{A,F} = \sum_{r=1}^{\infty} Z_r J_z^r. \quad (12)$$

As a function of the net interactions, the magnetic orders in the system are determined by the values of $\mu = \min\{\mathcal{J}_x^F, \mathcal{J}_x^A, \mathcal{J}_y^F, \mathcal{J}_y^A\}$

$$\mu = \begin{cases} \mathcal{J}_x^F \Rightarrow \text{Ferrom. order along } x; \\ \mathcal{J}_y^F \Rightarrow \text{Ferrom. order along } y; \\ \mathcal{J}_x^A \Rightarrow \text{Antiferrom. order along } x; \\ \mathcal{J}_y^A \Rightarrow \text{Antiferrom. order along } y. \end{cases} \quad (13)$$

It is interesting to observe that, in terms of the net interactions, one can immediately establish the presence or absence of frustration in the system: any frustration arising from the presence of competing interactions would imply that $\mu \neq -\sum_r Z_r |J_\alpha^r|$, with $\alpha=x,y$ depending on which of the two axes is characterized by a nonvanishing value of the magnetization. We remark that here and in the following we are not considering the particular situation in which a *saturation* occurs rather than a true ground state factorization: This instance will be discussed separately in Sec. IV D.

From now on, without loss of generality, we will specialize our analysis to the case of an antiferromagnetic or-

dering along the x direction. With trivial modifications, all the steps and results that will be obtained in the following hold as well in the remaining three cases of Eq. (13). At the end of the procedure we will present a summary table collecting the main results for all the four types of magnetic orders compatible with factorization.

Given an antiferromagnetic ordering along the x direction, and keeping in mind that in such case $\varphi_k = |k| \pi \forall k$, Eq. (7) implies that $M_y = 0$ while $M_k^x = \pm M_\perp \equiv \pm M_x$ with $M_x = M_\perp \geq 0$. The \pm sign reflects the fact that the antiferromagnetic order discriminates between two sublattices, each characterized by the opposite sign of the staggered magnetization along x . Consequently, the general condition Eq. (8) takes the form

$$0 = (\sin \theta M_z - \cos \theta M_x) \times [\cos \theta M_x \mathcal{J}_x^A - \sin \theta (M_z \mathcal{J}_z^F - h_f)], \quad (14)$$

that admits two solutions for θ ,

$$\tan \theta = \frac{M_x}{M_z}; \quad \tan \theta = \frac{\mathcal{J}_x^A M_x}{\mathcal{J}_z^F M_z - h_f}. \quad (15)$$

However, since the E-SQUO must be unique,²⁸ the two solutions must coincide. Factorization thus requires that

$$M_z = \frac{h_f}{\mathcal{J}_z^F - \mathcal{J}_x^A}. \quad (16)$$

Moreover, the requirement of a vanishing tangle (single-site entanglement) imposes

$$M_x = \frac{1}{2} \sqrt{1 - \frac{4h_f^2}{(\mathcal{J}_z^F - \mathcal{J}_x^A)^2}}. \quad (17)$$

Combining Eqs. (16) and (17) via Eq. (3) yields a closed expression for the phase θ as a function of the Hamiltonian parameters and of the factorizing field h_f

$$\cos \theta = \frac{2h_f}{\mathcal{J}_z^F - \mathcal{J}_x^A}. \quad (18)$$

Therefore, Eq. (18), together with the knowledge of $\varphi_k = \pi |k|$, once inserted into Eq. (2), determines, independently of the value of the magnetizations, the form of the E-SQUO at factorization:

$$\bar{O}_k = \cos \theta S_i^z + e^{i\varphi_k} \sin \theta S_i^x. \quad (19)$$

The form of the candidate factorized state $|\Psi_f\rangle$ is then readily determined by imposing that the action of the E-SQUO on all lattice sites leaves the ground state invariant

$$\otimes_k \bar{O}_k |\Psi_f\rangle = |\Psi_f\rangle. \quad (20)$$

From Eqs. (20) and (19) we find then that the candidate factorized ground state $|\Psi_f\rangle$ has to be a tensor product of single-site states that are the exact eigenstates of the operators \bar{O}_k with eigenvalue $1/2$

$$|\Psi_f\rangle = \otimes_k |\psi_k\rangle;$$

$$|\psi_k\rangle = \cos(\theta/2) |\uparrow_k\rangle + e^{i\varphi_k} \sin(\theta/2) |\downarrow_k\rangle. \quad (21)$$

Equation (21) expresses the general form that a factorized ground state must assume given an antiferromagnetic order along x . This result is independent on the actual values assumed by the staggered magnetizations M_α 's. We remark that in order to establish the general form of the candidate ground state it is essential to impose the vanishing of the EXE. In fact, without requiring it, the phase θ and the candidate factorized ground state become explicitly dependent on the magnetizations. Then, imposing the conditions for Eq. (21) to be an eigenstate of the Hamiltonian, one merely obtains a relation between the factorizing field h_f and the magnetizations M_α 's. If the analytic expression of at least one of the M_α 's is known, it is still possible to obtain an expression of the field h_f in terms of the Hamiltonian parameters. However, this actually occurs in few special, exactly solvable, cases (for instance, the XY model³³). Otherwise, in general one needs to resort to numerical evaluations of the magnetizations or introduce other approximations in the analysis. This problem is completely eliminated in the general analytic framework based on the invariance of the factorized ground states under the action of E-SQUOs and on the vanishing of the EXE at factorization.

Before proceeding further let us clarify a relevant point. Because of the even-odd symmetry of the energy spectra of the system, as elucidated also in Refs. 22 and 23, the assignment of one of the two different staggered magnetizations to each sublattice is arbitrary. According to this observation, one sees that, inverting the sign of the magnetization along the x direction on each site, all the conditions for factorization are still satisfied but the candidate ground state takes the form

$$|\Psi_f'\rangle = \otimes_k |\psi_k'\rangle;$$

$$|\psi_k'\rangle = \cos(\theta/2) |\uparrow_k\rangle + e^{i\varphi_k+1} \sin(\theta/2) |\downarrow_k\rangle. \quad (22)$$

Obviously the two states in Eqs. (21) and (22) are distinguishable and both $|\Psi_f\rangle$ and $|\Psi_f'\rangle$ are legitimate candidate ground states of the system, as well as general linear combinations of the two (the latter will be in general highly entangled). Here and in the following we assume to be working in a situation of broken symmetry, i.e., after that a small perturbing external field along the x direction has lifted the degeneracy between $|\Psi_f\rangle$ and $|\Psi_f'\rangle$, e.g., lowering the energy of the former and rising that of the latter. After a time long enough to ensure convergence to equilibrium, i.e., relaxation to the state $|\Psi_f\rangle$, the perturbation is switched off: in the thermodynamic limit, this ensures that the system will remain indefinitely in the state $|\Psi_f\rangle$.

Having determined the exact form of the candidate factorized ground state, the subsequent step concerns the determination of the conditions for its occurrence, i.e., the conditions under which a state of the form (21) is indeed the eigenstate of H , Eq. (6), with the lowest energy eigenvalue. To this aim, taking the value of the external field at the factorization point, $h = h_f$, it is useful to decompose the total Hamiltonian

as a sum of pairwise Hamiltonian terms $H_{\underline{i},\underline{j}}$, so that $H|_{h=h_f} = \sum_{\underline{i},\underline{j}} H_{\underline{i},\underline{j}}$, where each term $H_{\underline{i},\underline{j}}$ involves only the degrees of freedom of a single pair of spins

$$H_{\underline{i},\underline{j}} = J_x^r S_i^x S_j^x + J_y^r S_i^y S_j^y + J_z^r S_i^z S_j^z - h_f^r (S_i^z + S_j^z). \quad (23)$$

Here the quantity h_f^r plays the role in the ‘‘component’’ of the factorizing field that acts on the selected pair of spins and obeys the following relation:

$$2h_f^r = \cos \theta (J_z^r - (-1)^r J_x^r). \quad (24)$$

The above ensures that $h_f = \sum_r Z_r h_f^r$ satisfies Eq. (18). Proving that the candidate factorized ground state $|\Psi_f\rangle$ is an eigenstate of the total Hamiltonian H is equivalent to prove that it is a simultaneous eigenstate of all pair Hamiltonians $H_{\underline{i},\underline{j}}$, or, more precisely, that the projection of $|\Psi_f\rangle$ onto the subspace of two given spins \underline{i} and \underline{j} —which is still a pure state since $|\Psi_f\rangle$ is a tensor product of single-spin pure states—is an eigenstate of $H_{\underline{i},\underline{j}}$ for every pair $\{\underline{i},\underline{j}\}$. To proceed, we associate to each lattice site a set of orthogonal spin operators defined as follows:

$$\begin{aligned} A_i^x &= \cos \theta \cos \varphi_i S_i^x - \sin \theta S_i^z; \\ A_i^y &= \cos \varphi_i S_i^y; \\ A_i^z &= \sin \theta \cos \varphi_i S_i^x + \cos \theta S_i^z. \end{aligned} \quad (25)$$

It is immediate to observe that $A_k^z \equiv \bar{O}_k^z$. By inverting Eq. (25), we can conveniently re-express the standard spin operators as functions of the new set of operators $\{A_i^\alpha\}$

$$\begin{aligned} S_i^x &= \cos \varphi_i (A_i^x \cos \theta + A_i^z \sin \theta); \\ S_i^y &= A_i^y \cos \varphi_i; \\ S_i^z &= -A_i^x \sin \theta + A_i^z \cos \theta. \end{aligned} \quad (26)$$

Inserting Eq. (26) in Eq. (23) we obtain the expression of the pair Hamiltonian $H_{\underline{i},\underline{j}}$ as a function of the sets of operators $\{A_i^\alpha\}$ and $\{A_j^\alpha\}$

$$\begin{aligned} H_{\underline{i},\underline{j}} &= A_i^z A_j^z [\cos^2 \theta J_z^r + \sin^2 \theta J_x^r (-1)^r] - 2h_f^r \sin \theta \left[A_i^x \left(A_j^z - \frac{1}{2} \right) \right. \\ &\quad \left. + \left(A_i^z - \frac{1}{2} \right) A_j^x \right] + A_i^x A_j^x (\sin^2 \theta J_z^r + \cos^2 \theta (-1)^r J_x^r) \\ &\quad + A_i^y A_j^y (-1)^r - h_f^r \cos \theta (A_i^z + A_j^z), \end{aligned} \quad (27)$$

where we recall that r is the distance between sites \underline{i} and \underline{j} and that, in the presence of an antiferromagnetic order along the x direction, $\cos \varphi_i \cos \varphi_j = (-1)^r$. The spin-pair projection $|\psi_i\rangle|\psi_j\rangle$ of $|\Psi_f\rangle$ is an eigenstate of the pair Hamiltonian $H_{\underline{i},\underline{j}}$ either if all terms in Eq. (27) admit $|\psi_i\rangle|\psi_j\rangle$ as an eigenstate or if they annihilate it. By construction, recalling that $A_i^z \equiv \bar{O}_i^z$ and that $|\psi_i\rangle$ is the eigenstate of A_i^z with eigenvalue

equal to $1/2$, the spin-pair projection of $|\Psi_f\rangle$ is an eigenstate of the pair Hamiltonian if the following condition holds:

$$\cos^2 \theta J_x^r + (-1)^r \sin^2 \theta J_z^r - J_x^r = 0. \quad (28)$$

For general models of the type (6) with a given, arbitrary, maximum spatial range of interaction s , Eq. (28) admits the following solution:

$$\cos^2 \theta = \frac{J_y^r - (-1)^r J_z^r}{J_x^r - (-1)^r J_z^r}, \quad (29)$$

for all distances $r \leq s$, i.e., for all distances associated with nonvanishing couplings (we recall that $J_\alpha^r = 0 \forall \alpha$ and $\forall r \geq s+1$). The set of Eq. (29) determines the conditions that must be satisfied simultaneously by the phase θ , which is unique, in order for $|\Psi_f\rangle$ to be an eigenstate of the total Hamiltonian (6). Equation (29) discriminates quite clearly between short-range models, i.e., models with only one nonvanishing coupling at $r=s=1$ (models with nearest-neighbor interactions) and all other possible models containing finite- or infinite-range interaction terms. Specifically, models with only nearest-neighbor interactions are characterized by the fact that Eq. (29) reduce to a single condition and hence if the value of the right-hand side (rhs) of Eq. (29) falls in the interval $[0,1]$ (associated to the permitted values of $\cos^2 \theta$ in terms of the interaction parameters), one can immediately conclude that the models under investigation admit a factorized eigenstate. On the other hand, for models containing interaction terms of longer range—so that Eq. (29) include two or more conditions—factorized energy eigenstates are allowed if and only if the rhs of all conditions in the set Eq. (29) take values in the interval $[0,1]$ and, moreover, they all coincide.

Summing term by term over the index r all the relations in Eq. (28), taking into account Eq. (18), and solving for h_f , one eventually obtains the exact expression of the factorizing field as a function of the net interactions

$$h_f = \frac{1}{2} \sqrt{(\mathcal{J}_x^A - \mathcal{J}_z^F)(\mathcal{J}_y^A - \mathcal{J}_z^F)}. \quad (30)$$

We remark that Eq. (30), which was derived in Ref. 27 using some unnecessary auxiliary assumptions, is completely general and holds for lattices of arbitrary spatial dimension and for spin-spin interactions of arbitrary range. Accordingly, the angle θ that determines the direction of the E-SQUO can be also expressed as a function of the net interactions as follows:

$$\cos \theta = \sqrt{\frac{\mathcal{J}_y^A - \mathcal{J}_z^F}{\mathcal{J}_x^A - \mathcal{J}_z^F}}. \quad (31)$$

In the case of a maximum range of interaction $s \geq 2$, relation (31) for the net interactions is a necessary but not sufficient condition for factorization, and further use of Eqs. (28) and (29) is needed, as we will show with explicit examples in Secs. VI and VIII.

We are finally left with the problem of establishing conditions for a factorized energy eigenstate $|\Psi_f\rangle$ to be indeed a ground state of the system. A very simple sufficient but not

TABLE I. Summary of results for the four magnetic orderings [Eq. (13)] compatible with ground state factorization.

Magnetic order	$\cos^2 \theta$	Factorizing field h_f	Single-spin state $ \psi_k\rangle$
$\mu = \mathcal{J}_x^F$	$\frac{J_x^r - J_z^r}{J_x^r - J_y^r}$	$\frac{1}{2} \sqrt{(\mathcal{J}_x^F - \mathcal{J}_z^F)(\mathcal{J}_y^F - \mathcal{J}_z^F)}$	$\cos(\theta/2) \uparrow_k\rangle + \sin(\theta/2) \downarrow_k\rangle$
$\mu = \mathcal{J}_x^A$	$\frac{J_y^r - (-1)^r J_z^r}{J_x^r - (-1)^r J_z^r}$	$\frac{1}{2} \sqrt{(\mathcal{J}_x^A - \mathcal{J}_z^A)(\mathcal{J}_y^A - \mathcal{J}_z^A)}$	$\cos(\theta/2) \uparrow_k\rangle + (-1)^{ k } \sin(\theta/2) \downarrow_k\rangle$
$\mu = \mathcal{J}_y^F$	$\frac{J_x^r - J_z^r}{J_x^r - (-1)^r J_z^r}$	$\frac{1}{2} \sqrt{(\mathcal{J}_x^F - \mathcal{J}_z^F)(\mathcal{J}_y^F - \mathcal{J}_z^F)}$	$\cos(\theta/2) \uparrow_k\rangle + i \sin(\theta/2) \downarrow_k\rangle$
$\mu = \mathcal{J}_y^A$	$\frac{J_x^r - (-1)^r J_z^r}{J_y^r - (-1)^r J_z^r}$	$\frac{1}{2} \sqrt{(\mathcal{J}_x^A - \mathcal{J}_z^A)(\mathcal{J}_y^A - \mathcal{J}_z^A)}$	$\cos(\theta/2) \uparrow_k\rangle + (-1)^{ k } i \sin(\theta/2) \downarrow_k\rangle$

necessary condition is that the spin-pair projection of $|\Psi_f\rangle$ onto the subspace of a pair of spins be the simultaneous ground state of every pair Hamiltonian H_{ij} . In fact, given the relation existing between all the pair Hamiltonians H_{ij} in Eq. (23) and the total Hamiltonian H in Eq. (6), it follows that the simultaneous ground state of all pair Hamiltonians H_{ij} is also ground state of H . To proceed, let us re-express the pair Hamiltonians (27) in matrix form in the basis spanned by the eigenstates of the operators $A_i^z \otimes A_j^z$. One has

$$H_{ij} = \begin{pmatrix} \alpha_r - h_f^r & 0 & 0 & 0 \\ 0 & -\alpha_r & J_y^r/2 & \beta_r \\ 0 & J_y^r/2 & -\alpha_r & -(-1)^r \beta_r \\ 0 & \beta_r & -(-1)^r \beta_r & \alpha_r + h_f^r \end{pmatrix}, \quad (32)$$

where $\alpha_r = \frac{1}{4}[\cos^2 \theta J_z^r + (-1)^r \sin^2 \theta J_x^r]$ and $\beta_r = h_f^r \sin \theta$. Making use of Eqs. (24) and (31) the eigenvalues of the matrix Eq. (32) can be put in the form

$$\begin{aligned} \varepsilon_0 &= \frac{1}{8}[3(-1)^r J_x^r - J_z^r - (J_z^r - (-1)^r J_x^r) \cos(2\theta)], \\ \varepsilon_1 &= \frac{1}{8}[3(-1)^r J_x^r - J_z^r - (J_z^r - (-1)^r J_x^r) \cos(2\theta)], \\ \varepsilon_2 &= \frac{1}{8}[-3((-1)^r J_x^r + J_z^r) + (J_z^r - (-1)^r J_x^r) \cos(2\theta)], \\ \varepsilon_3 &= \frac{1}{8}[-3(-1)^r J_x^r + 5J_z^r + (J_z^r - (-1)^r J_x^r) \cos(2\theta)]. \end{aligned} \quad (33)$$

The eigenvalue ε_0 is the one associated to the projection $|\psi_i\rangle|\psi_j\rangle$ of the factorized eigenstate $|\Psi_f\rangle$ onto the four-dimensional Hilbert space associated to the pair of spins $\{S_i^z, S_j^z\}$. Therefore, the spin-pair projection is the ground state of the pair Hamiltonian if $\varepsilon_0 \leq \{\varepsilon_1, \varepsilon_2, \varepsilon_3\}$. Imposing this condition yields the following inequalities:

$$(J_x^r + J_y^r)[J_x^r - (-1)^r J_z^r] \geq 0; \quad (34)$$

$$(-1)^r J_x^r - J_z^r \leq 0. \quad (35)$$

Notably, these inequalities are automatically satisfied for any interacting spin system that is not frustrated and that verifies all of the Eq. (29). Namely, for every even value of the distance r in the interaction range ($r \leq s$) Eq. (35) implies

that the denominator in the corresponding Eq. (29) is non-positive. Therefore, an acceptable value of $\cos^2 \theta$ can be obtained only if also the numerator is nonpositive and exceeds or equals the denominator. These conditions in turn imply the order relation, $J_x^r \leq J_y^r$. On the other hand, comparing Eqs. (34) and (35), one has that $J_x^r \leq -J_y^r$. Therefore, comparing the two order relations yields finally $J_x^r \leq -|J_y^r|$ (r even). This condition is always verified in systems with an antiferromagnetic order along the x direction and in absence of frustration and therefore the projection of the factorized energy eigenstate on the Hilbert space of every pair of spins is indeed the ground state of every pair Hamiltonian. On the other hand, in the case of odd r , Eq. (35) implies that the denominator of Eq. (29) is non-negative and, similarly to the former case, the numerator must be non-negative and not exceeding the denominator. Hence we obtain $J_x^r \geq J_y^r$ while from Eq. (34) we recover $J_x^r \geq -J_y^r$ that, in turn, implies $J_x^r \geq |J_y^r|$. Again, such inequalities are always verified in the presence of an antiferromagnetic order and in the absence of frustration.

Collecting all these results, we have proved that the following holds:

Theorem. For any cooperative system of spin-1/2 particles described by Hamiltonians H of the type [Eq. (6)], characterized by an antiferromagnetic order along the x axis as emerging from Eq. (13) and in the absence of frustration, the simultaneous verification of all Eqs. (28) is necessary and sufficient for the fully factorized state Eq. (21) to be the exact ground state of H when the external magnetic field takes the value $h = h_f$ determined by Eq. (30).

This central result holds as well, with obvious modifications, when one considers the other different ordered phases that form the set identified in Eq. (13). In Table I we summarize and compare results for each of the four different possibilities.

D. Factorization, balancing, and saturation

Before moving to apply the general method to specific models and examples of conceptual and physical relevance, we discuss briefly the meaning of factorization and its marked differences with the phenomenon of ‘‘saturation’’ (see below). As we have seen, and as it will appear even clearer in the discussion of the examples in the following sections, the physical mechanism of ground state factorization in quantum spin systems is due to a delicate kind of ‘‘balancing’’ between the coupling strengths that regulate the intensity (and range) of the interactions and the aligning effect of the external field, that tend to orient all spins along a

given direction and to destroy all quantum correlations. The remarkable aspect of factorization is that then it occurs, according to well-defined conditions and constraints, at precisely defined, finite values of the couplings and of the fields in an ordered (or symmetry broken) phase. This means that factorization occurs when the system is relatively strongly interacting and the external aligning field is relatively weak. Moreover, we will see that the factorization point is always a precursor from below (from the ordered phase) the quantum critical point, as first observed for the XYZ model with nearest-neighbor interactions.²¹

Saturation is the phenomenon of ground state factorization that occurs trivially when the value of the external field grows unboundedly compared to all other Hamiltonian parameters. Therefore its aligning effect on the spins prevails against all other effects and quantum correlations are suppressed. The main physical difference between proper factorization and saturation is then clear and is reflected at the level of the Hilbert space of states. Namely, suppose that the system under study admits a fully factorized state that is the true ground state of the system at $h=h_f$. Then, when one moves away from the factorizing field, i.e., when $h-h_f=\epsilon \neq 0$, the factorized state ceases to be an eigenstate of the Hamiltonian. On the contrary, in the presence of saturation, the trivially ensuing factorized state is always an eigenstate of the Hamiltonian and remains the ground state of the system when perturbing the value of the external field h .

Let us formalize the above discussion. Consider a system that admits a fully factorized ground state. In this case the pair Hamiltonian in Eq. (27) admits as eigenstate a factorized spin-pair state. However, Eq. (27) is the expression of the pair Hamiltonian only at $h=h_f$. If we consider a value of the external field different from the factorizing field we must include in Eq. (27) a term proportional to $(A_x^i - A_y^i) \sin \theta (h - h_f)$. Obviously, for nonvanishing values of $\sin \theta$ the presence of such term prevents the factorized state from being an eigenstate of the Hamiltonian of the system. On the contrary, if $\sin \theta=0$ and hence if $\bar{O}_k \equiv S_k^z \nabla_k$ the extra Hamiltonian term vanishes and the factorized state $\otimes_k |\uparrow\rangle_k$ remains an energy eigenstate of the system for all values of the external field. This result can be understood from a different point of view. When $\theta=0$, from Eq. (29) we immediately obtain that $J_x^r = J_y^r$, which implies that the total magnetization along the z axis is preserved, $[H, \sum_k S_k^z] = 0$. Therefore the Hamiltonian of the system and the total magnetization operator admit a complete set of common eigenstates, discriminated by the eigenvalue of the total magnetization: the factorized state is the one (and only one) characterized by the maximum eigenvalue.

We now move on to show that the factorized eigenstate, in the case of saturation, is the system's ground state in an infinite range of values of the external field. Here and in the following we recall that since the external field is directed along the conventional z direction, only saturation with spin alignment along the z axis is allowed. At very low values of h the ground state of the system will possess a small total magnetization along the field direction. However, as h increases, also the total ground state magnetization along the z direction will increase until all spins align with the field and

saturation occurs. By increasing h further, it is not possible for the system to evolve in a state with higher values of the magnetization along the field direction. Hence, the factorized state remains the ground state of the system for all values of the external field $h \geq h_s$, where by h_s we denote the value of the field for which the system reaches saturation ("saturating field"). Let us consider the matrix representation, similarly to Eq. (32), of the pair Hamiltonian at arbitrary values of h . Taking into account the condition $\sin \theta=0$ we have

$$H_{ij} = \begin{pmatrix} J_z^r/4 - h^r & 0 & 0 & 0 \\ 0 & -J_z^r/4_r & J_y^r/2 & 0 \\ 0 & J_y^r/2 & -J_z^r/4_r & 0 \\ 0 & 0 & 0 & J_z^r/4_r + h_f^r \end{pmatrix}. \quad (36)$$

It is immediate to verify that if $h^r \geq |J_x^r|/2 + J_z^r/2 = h_s^r$, the projection of the factorized state onto the considered pair of spins is associated to the lowest energy. Resumming over all values of the spatial range index r and taking into account the coordination number Z_r of the lattice, we have that the factorized state is the ground state of the total system if

$$h \geq h_s = \frac{1}{2} \left(\sum_r Z_r |J_x^r| + \sum_r Z_r J_z^r \right). \quad (37)$$

Equation (37) is the rigorous condition for saturation. We notice that it coincides with Eq. (30) in the limit $J_y^r \rightarrow J_x^r$, meaning that in this simple instance no ground state factorization occurs other than saturation.

In the following sections we apply the general theory of factorization to different quantum spin models. We will derive a series of exact results concerning the occurrence of factorized ground states in systems with various types of two-body interactions of different spatial ranges defined on regular lattices of arbitrary spatial dimensionality. The general method enables to determine many exact factorized ground state solutions as well as the existence and the nature of ordered phases in models that are, in general, nonexactly solvable. Moreover, it allows to recover quite straightforwardly the existing analytical and numerical results. In the process, we will come to appreciate that ground state factorization is a phenomenon more common than previously believed. Determining the existence of exact factorized solutions in nonexactly solvable models should in turn allow to envisage controlled approximation schemes, e.g., perturbative or variational, to investigate the physics of nonexactly solvable quantum spin models in the vicinity of quantum factorization points.

V. MODELS WITH SHORT-RANGE INTERACTIONS

In this and in the following sections we will consider quantum spin models of the XYZ type Eq. (6) defined on regular lattices of arbitrary dimension. Let us first consider models with short-range interactions including only nearest-neighbor couplings

$$J_\alpha^1 \equiv J_\alpha, \quad J_\alpha^r = 0, \quad \forall r \geq 2. \quad (38)$$

As in Sec. IV we restrict ourselves to the case in which such models are defined on regular lattices of a generic dimension

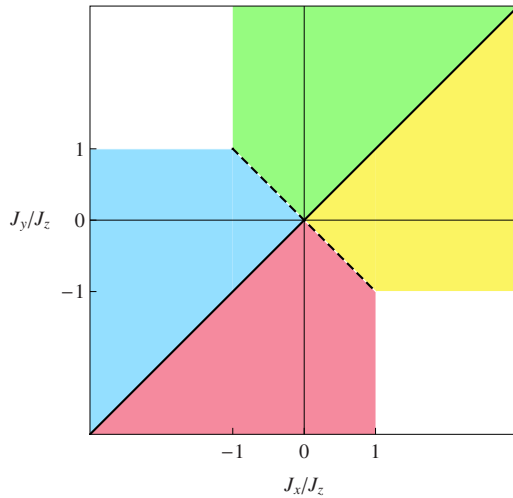


FIG. 1. (Color online) Diagram of ground state factorization as a function of the ratios J_x/J_z and J_y/J_z . The coupling J_z is set to be positive for reference. Analogous results hold in the case $J_z < 0$. Blank regions: no factorization allowed. Rightmost (yellow) shaded region: presence of a fully factorized ground state supporting an antiferromagnetic order along the x direction. Leftmost (light blue) shaded region: fully factorized ground state with a ferromagnetic order along x . Bottommost (light red) shaded region: Fully factorized ground state with a ferromagnetic order along the y direction. Topmost (light green) shaded region: fully factorized ground state with an antiferromagnetic order along y . The solid line $J_x = J_y$ corresponds to models that exhibit saturation rather than true factorization; the dashed line $J_y = -J_x$ accommodates for models with unresolved superpositions of two fully factorized ground states each one supporting a different magnetic order. Either one of the two possible ground states is then “chosen” by the system depending on the way the symmetry is broken, see text for further details. All plotted quantities are dimensionless.

sion, whose geometry does not induce any frustration, i.e., in which any closed loop is characterized by an even number of spins. The absence of geometrical frustration together with the fact that all the couplings beyond the nearest-neighbor spins vanish, ensure that it is always possible for the system to satisfy all the conditions on the net magnetic interactions. Therefore, as shown in Sec. IV, if the rhs of Eq. (29)—or, better, if the rhs of the equation relative to each possible magnetic order (See Table I) takes an acceptable value ($0 \leq \text{rhs} \leq 1$)—then the system admits a fully factorized ground state. In the case of antiferromagnetic ordering along the x direction, which is obtained if $J_x \geq |J_y|$, from Eq. (29) it follows that a factorized ground state exists if $J_y \leq -J_z$. Analogous conditions are obtained for the other types of magnetic orders compatible with full ground state separability. The results are summarized in Fig. 1, where J_z is set assume positive values for reference. A very similar diagram of factorization holds in the case $J_z < 0$.

As one can see from Fig. 1, the type of magnetic order corresponding to the factorized ground state determines four different regions in the space of the Hamiltonian parameters (one for each different ordering) associated to the existence of a factorized ground state. The four different domains of the interaction parameters are separated by two bisectrices

that individuate special cases. The line $J_x = J_y$ is constituted by the set of points in which saturation occurs in place of genuine factorization (see Sec. IV D). On the other hand, the line $J_x = -J_y$, $-1 \leq J_x/J_z \leq 1$, corresponds to models that, for a given value of the factorizing field h_f and of the E-SQUO orientation θ , admit two degenerate, but distinct factorized states. The choice of the ground state is then determined by the usual mechanisms of symmetry breaking: if an infinitesimal magnetic field is applied in the xy plane, the axis of magnetic alignment in the ground state is determined by the order in which the two limits $h_x \rightarrow 0$ and $h_y \rightarrow 0$ are realized.

It is important to observe that all the shaded regions of Fig. 1 correspond to exact analytical ground state solutions of the investigated short-range models, which are, in general, nonexactly solvable. The exact, fully factorized ground states are tensor products of the form reported in the fourth column of Table I, in which the value of the orientation parameter θ of the E-SQUO is retrieved by solving the equation in the second column of Table I. Obviously, such an exact solution holds only at the factorizing field $h = h_f$. In the case of antiferromagnetic order either along the x or the y direction, the latter is given by (see Table I)

$$h_f = \frac{Z_1}{2} \sqrt{(J_x + J_z)(J_y + J_z)}, \quad (39)$$

while in the case of a ferromagnetic phase, again unrespectfully if along x or along y , it reads

$$h_f = \frac{Z_1}{2} \sqrt{(J_x - J_z)(J_y - J_z)}. \quad (40)$$

Given that the ground state is known exactly at the factorization point, all the relevant physical observables can be evaluated straightforwardly. For instance, the ground state energy density at factorization reads

$$\frac{E}{N} = -\frac{Z_1}{8} (J_x + J_y + J_z) \quad (41)$$

in the presence of an antiferromagnetic ordering, while in the ferromagnetic case it is

$$\frac{E}{N} = \frac{Z_1}{8} (J_x + J_y - J_z). \quad (42)$$

Both the factorizing field and the ground state energy, unlike the E-SQUO orientation θ and the expression of the factorized ground states, are functions of the number of nearest neighbors per site (the coordination number Z_1 , where the index 1 denotes the nearest-neighbor range of the interactions). Hence, they depend on the geometry and the spatial dimension of the lattice. To begin with, let us consider one-dimensional lattices (spin chains, $D=1$), for which the coordination number $Z_1=2$. Substituting this value in the previous equations, we immediately recover, among others, the value of the factorizing field and the ground state energy obtained analytically by Kurmann *et al.* for the XYZ spin chain using the direct method.²⁰ Kurmann *et al.* had to restrict their investigation to coupling constants J_α taking values in the interval $[0,1]$, thus establishing ground state factorization only in a restricted set of conditions. Instead, the

general method allows to assess the occurrence of factorized ground states associated to different types of magnetic orderings in the entire region of the Hamiltonian parameters.

One of the most important advantages of the general method is that it is easily applicable irrespective of the spatial dimensionality, while the direct method becomes increasingly difficult to apply with growing spatial dimensions of the lattice. Numerical techniques can overcome some of the limits of the direct method, although they fall short of the power and extension of the general analytic method. The most important numerical result has been obtained by applying quantum Monte Carlo techniques to the study of the XYZ model in $D=2$ space dimensions (square lattice).²¹ Applying the present method to the XYZ model on the square lattice allows not only to immediately reobtain analytically the previous numerical findings but also, again, to extend the investigation to the entire space of the Hamiltonian parameters by simply taking into account that for the square lattice $Z_1=4$. Moreover, the flexibility of the general method allows to include in the analysis of different planar models. For instance, considering models defined on planar hexagonal lattices, the previous analysis needs to be modified only in that the value of the coordination number, in this case is $Z_1=3$.

Let us now move to $D=3$ and investigate ground state factorization in nearest-neighbor XYZ models on three-dimensional regular lattices, for which there were so far no results (apart the preliminary ones obtained in our previous work²⁷) either analytic or numerical (such a task would be extremely demanding if approached either via the direct method or via numerical techniques). Resorting to the general method, we can instead fully characterize the factorized ground state and the associated physical quantities just by entering the correct value of the coordination number, e.g., $Z_1=6$ for a simple cubic lattice. Obviously, the results extend straightforwardly also for models defined on lattices of arbitrary higher dimension $D>3$.

VI. MODELS WITH FINITE- AND LONG-RANGE INTERACTIONS

The analytic method can be applied with minor complications to models with interactions of longer spatial range. As already mentioned in Sec. IV, concerning ground state factorization, the main difference between models with short- and finite-range interactions is that for the latter there exist more than one equation in the set Eq. (29). Each of these equations is associated to a different value of the range $r \leq s$, where s is the maximum interaction range, that is the maximum distance between two directly interacting spins: all the couplings vanish for pairs of spins with interspin distance greater or equal to $s+1$.

Clearly, the fact that all the equations have to be solved simultaneously yields tighter conditions on factorizability compared to the case of models with nearest-neighbor interactions. Namely, it is not sufficient that the rhs of each Eq. (29) takes values in the interval $[0,1]$. It is also necessary to require that all these values coincide. This constraint yields a set of further conditions that must be satisfied by all the nonvanishing couplings. For instance, let us suppose that the

system is in an antiferromagnetic ordered phase along the x direction. Labeling by c the value of $\cos^2 \theta$ and imposing that for every r the rhs of Eq. (29) must equate c , we find that

$$J_y^r = cJ_x^r + (-1)^r(1-c)J_z^r \quad \forall r \leq s, \quad (43)$$

where, to ensure the absence of frustration, J_x^r must obey the following inequality: $(-1)^r J_x^r \leq J_z^r(c-1)/(1+c) \quad \forall r \leq s$. Analogously, for an antiferromagnetic order along y

$$J_x^r = cJ_y^r + (-1)^r(1-c)J_z^r \quad \forall r \leq s, \quad (44)$$

and to exclude frustration we must also have that $(-1)^r J_y^r \leq J_z^r(c-1)/(1+c) \quad \forall r \leq s$. In the presence of a ferromagnetic phase, respectively, for an ordering along x and along y , the constraints and the no-frustration condition become

$$J_y^r = cJ_x^r + (1-c)J_z^r \quad J_x^r \leq \frac{c-1}{1+c}J_z^r \quad \forall r \leq s; \quad (45)$$

$$J_x^r = cJ_y^r + (1-c)J_z^r \quad J_y^r \leq \frac{c-1}{1+c}J_z^r \quad \forall r \leq s. \quad (46)$$

Equations (43)–(46) generalize the instance analyzed in Ref. 27, in which we limited the analysis to the case of vanishing J_z that, according to Eqs. (43)–(46), implies $c=J_x^r/J_y^r$ for all $r \leq s$.

Especially in the presence of a ferromagnetic order in the lattice, Eqs. (45) and (46) allow us to simplify the expressions of both the factorizing field and the energy per site. Namely, taking into account the definition of the ferromagnetic net interactions Eq. (11) and the expression of the factorizing field in the presence of a ferromagnetic order (see Table I), we have

$$h_f = \sqrt{c}(\mathcal{J}_x^F - \mathcal{J}_z^F),$$

$$h_f = \sqrt{c}(\mathcal{J}_y^F - \mathcal{J}_z^F), \quad (47)$$

respectively, for an order along the x and the y directions. Similarly, for the energy density we obtain

$$\frac{E}{N} = (1+c)\mathcal{J}_x^F - c\mathcal{J}_z^F,$$

$$\frac{E}{N} = (1+c)\mathcal{J}_y^F - c\mathcal{J}_z^F. \quad (48)$$

We now discuss a specific example (out of many possible ones) which demonstrates the power of the analytic method in conditions where the more conventional direct approach based on the factorized ansatz of Refs. 20 and 23 is completely ineffective without the supplement of a remarkable intuition in guessing the correct forms of the possible factorized ground states. Let us consider a XYZ-type spin model defined on a spatially isotropic cubic lattice of arbitrary size, possessing nearest-neighbor and next-nearest-neighbor interactions, and admitting arbitrarily different couplings along the x , y , and z directions. The coordination numbers associated to the two types of interactions can be straightforwardly computed from the geometry of the problem and are $Z_1=6$ and $Z_2=18$. Suppose the model is deduced from an explicit experimental realization of a spin lattice and we are provided

with explicit values of the various interaction strengths. For example, $J_x^1=1$, $J_y^1=0.3$, $J_z^1=0.4$, $J_x^2=-0.6$, $J_y^2=-0.25$, $J_z^2=0.1$. The application of our “on-demand” ground state factorization search engine is now immediate. From Eq. (13) we have that the candidate factorized state must possess antiferromagnetic order along the x direction. Therefore the general conditions for the existence of a factorization point, as determined by Eq. (29), can be summarized as follows:

$$\cos^2 \theta = \frac{J_y^1 + J_z^1}{J_x^1 + J_x^2} = \frac{J_y^2 - J_z^2}{J_y^1 - J_z^1} = \frac{J_y^1 + J_z^1 - 3(J_y^2 - J_z^2)}{J_x^1 + J_x^2 - 3(J_x^2 - J_x^1)}. \quad (49)$$

This condition must hold together with the frustration-free constraint. It is readily verified that $\cos^2 \theta = 0.5$ provides a solution to the combined set of necessary and sufficient conditions for ground state factorization. Therefore if the experimentalist tunes the external field h at the factorizing value $h_f \approx 7.425$, obtained from Eq. (30), the engineered cubic spin lattice system will relax in a completely factorized ground state of the form given in Table I (second row, last column) with $\theta = \arccos(\sqrt{0.5})$.

Many other applications can be considered to models with arbitrary spin-spin interactions of longer range, and they can be treated with the same simplicity within the framework of the general analytic method. For instance, a very interesting example of a model with infinite-range interactions will be treated in the next section. However, before moving to the study of this case, we should comment on the important issue of the interplay between factorization and frustration in quantum spin systems with multiple spatial scales of interaction.

The investigation of general models including many interaction terms of different spatial ranges needs to be carried out with particular care, because the interplay between the different interactions can lead in general to important effects of frustration that tend to suppress the occurrence of ground state factorization. The very delicate and tricky nature of the problem is at the origin of a recent incorrect prediction about the existence of factorized ground states in one-dimensional XYZ models on finite rings with long-range interactions, obtained exploiting the direct method.³⁴ In Ref. 34 Giorgi, resorting to the direct method, concludes that all the factorized energy eigenstates in one-dimensional long-range XYZ models, with interaction terms of spatial ranges that are in integer ratio with the total number of sites, are also the states of lowest energy. However, the proof of this statement obtained using only the direct method requires that there must be no frustration in the system.²⁰ Unfortunately, the interplay between the interactions of different spatial range can in general introduce frustration effects (e.g., in the case of antiferromagnetic nearest-neighbor and next-to-nearest-neighbor interactions, and so on). The existence of these effects nullifies all proofs, based on the direct method, of the existence of fully separable ground states. In fact, immediate counterexamples can be given of fully factorized energy eigenstates that are not ground states. Let us consider, for instance, an XY model on a finite ring of six spins with nearest-neighbor and next-to-nearest-neighbor antiferromagnetic interactions, and $J_x^1=1$, $J_y^1=0.3$, $J_x^2=0.6$, $J_y^2=0.18$. Following Ref. 34,

this model should admit a factorized ground state. In fact, a factorized energy eigenstate with antiferromagnetic order does indeed exist, with an energy $E = -0.78$. However, solving the model by exact diagonalization yields that the lowest energy is $E \approx -1.11$ and that the associated ground state is entangled. Essentially the same type of counterarguments nullifies a recent claim that the factorized energy eigenstates are the factorized ground states of mixed spin models of ferromagnetism of the XYZ type.³⁵ A general analysis of ground state factorization in ferrimagnetic models with mixed spin-1/2-spin-1 interactions will be presented elsewhere,³⁶ based on a proper extension of the formalism of SQUOs to include spin-1 systems, as sketched in the final part of Ref. 28.

In conclusion, the study of factorization in quantum spin models with many different finite- and long-range interaction terms requires a very careful analysis and the use of the general analytic method whenever frustration effects are present. A rigorous and systematic study of the crucial (and subtle) interplay between frustration and factorization in quantum spin systems will be the subject of a forthcoming paper.³⁷

VII. LIPKIN-MESHKOV-GLICK MODEL

A very interesting limit of the cases analyzed in Sec. VI is given by models with infinite range interactions, such as the fully connected or Lipkin-Meshkov-Glick (LMG) model,³⁸ extensively studied in condensed matter physics,^{26,39,40} which is described by the following Hamiltonian

$$H = -\frac{1}{4(N-1)} \sum_{i,j} (S_i^x S_j^x + \Delta S_i^y S_j^y) - \frac{h}{2} \sum_i S_i^z, \quad (50)$$

with $0 \leq \Delta \leq 1$. The prefactor $1/4(N-1)$ (with N denoting the total number of spins) ensures the linear divergence of the ground state energy as N increases. Let us remark that normalizing the interaction part of the Lipkin-Meshkov-Glick Hamiltonian requires some care: being a connected interaction, it scales as $N \times (N-1)$, i.e., as the product of the total number of spins and the number of pairs of spins. Therefore, to ensure that the interaction energy is extensive, i.e., scales with N , the interaction part of the Hamiltonian must be normalized by $N-1$. Usually, for calculational ease, the interaction part is normalized by N , so that it scales as $N-1$. Using this convention is strictly speaking incorrect, but is clearly harmless for large N and in the thermodynamic limit. For instance, concerning the separability of the ground state, it introduces a slight, spurious N dependence of the factorization point through the multiplicative factor $(N-1)/N$, and the error vanishes in the thermodynamic limit. However, on fundamental physical grounds, the factorization points of translationally invariant systems, if they exist, must be independent on the size of the system, and must take the same value both at finite N and in the thermodynamic limit. Applying the Kurmann-Thomas-Müller factorized ansatz²⁰ and the $1/N$ normalization, Dusuel and Vidal²⁶ obtained an analytic expression of the factorizing field for the LMG model that is N dependent through the multiplicative factor

$(N-1)/N$. Although defined according to an anomalous convention, this result is essentially exact in the limit of large N .

We first observe that the LMG model in Eq. (50) can be obtained as the limiting case of a generic model described by Eq. (6) assuming that the range of interactions diverges (i.e., $s \rightarrow \infty$) while the individual strengths become independent on the distance ($J'_\alpha = J_\alpha$), scale with $N(J_\alpha \propto 1/N)$, and vanish along the z direction ($J_z = 0$). Therefore, assuming $J'_x = -2/N$, $J'_y = -2\Delta/N$, and $J_z = 0$ in Eq. (6) we recover Eq. (50).

Because of the sign of the interactions and of the range of values that can be assumed by Δ , we immediately obtain that the energy per site Eq. (10) is minimized by a state possessing ferromagnetic order along the x direction. Moreover, taking into account that the coupling strengths are proportional to the ratio $1/N$, we have that the net interactions converge to finite values in the thermodynamic limit: $\mathcal{J}_x^f \rightarrow -2$, $\mathcal{J}_y^f \rightarrow -2\Delta$. It is then rather straightforward to apply the analytic method to the LMG model and hence prove, exactly, that the ground state is fully factorized at the factorizing field $h_f = \sqrt{\Delta}$, which is, correctly, independent on N . The form of the fully separable ground state is the tensor product of local states of the form $|\psi_k\rangle = \cos(\theta/2)|\uparrow_k\rangle + \sin(\theta/2)|\downarrow_k\rangle$ with $\theta = \arccos(\sqrt{\Delta})$ and the energy density reads $E/N = -(1 + \Delta)/4$. These results are in agreement with those obtained, using the direct method, by Dusuel and Vidal,²⁶ modulo a proper normalization factor.

VIII. MODELS WITH SPATIAL ANISOTROPIES

The versatility and generality of the analytic method can be demonstrated further by considering extensions of the translationally invariant models discussed in the previous sections. In fact, till now, we have always considered systems in which the coupling amplitudes depend only on the distance between the spins involved. In the present subsection we shall focus instead on models which contemplate the possibility of spatial anisotropies, i.e., given the spin S_i associated to site i , the interaction coupling with spin S_j associated to site j depends not only on the distance $r = |i - j|$ but also on the location of site j relative to site i .

To simplify the notations, the physical analysis, and the number of possible cases that need to be considered, we limit ourselves to models with short-range interactions, i.e., with all the couplings vanishing for $r = |i - j| \geq 2$. We will comment briefly on general models with spatial anisotropies and interactions of arbitrary range at the end of this section. Let us assume that for each site i the total number of nearest neighbors is $Z_1 = Z_1^{(1)} + Z_1^{(2)}$, where $Z_1^{(1)}$ is the number of nearest neighbors whose coupling strength with S_i takes a certain value f_α , and $Z_1^{(2)}$ is the number of nearest neighbors whose coupling with S_i is given by a different value g_α . Obviously, we could consider situations more complicated at will, with an arbitrary number of n different types of nearest neighbors. For the given example, the system Hamiltonian reads

$$H = 1/2 \sum_i \left[\left(\sum_{k_1} f_x S_i^x S_{k_1}^x + f_y S_i^y S_{k_1}^y + f_z S_i^z S_{k_1}^z \right) + \left(\sum_{k_2} g_x S_i^x S_{k_2}^x + g_y S_i^y S_{k_2}^y + g_z S_i^z S_{k_2}^z \right) \right] - 2h S_i^z, \quad (51)$$

where the index k_1 runs over the first $Z_1^{(1)}$ nearest neighbors,

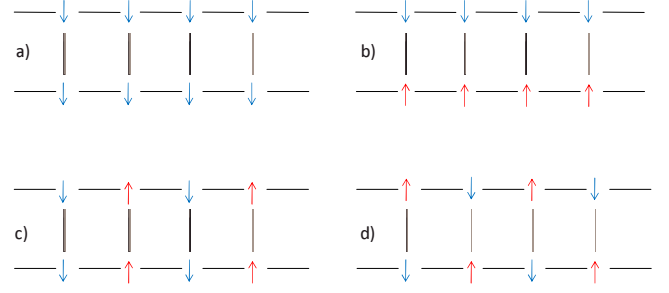


FIG. 2. (Color online) Summary of the possible magnetic arrangements along a single direction (x or y) characterizing the candidate-factorized ground states of models with spatially anisotropic interactions. The case considered corresponds to a ladder of two coupled one-dimensional spin chains with coordination numbers $Z_1^{(1)} = 2$ and $Z_1^{(2)} = 1$. Topmost row: (a) parallel and (b) antiparallel ferromagnetic orders. Bottommost row: (c) parallel and (d) antiparallel antiferromagnetic orders.

and the index k_2 runs over the remaining $Z_1^{(2)}$ nearest neighbors for each spin S_i . According to the different values of $Z_1^{(1)}$ and $Z_1^{(2)}$ this Hamiltonian describes various possible models. For instance, if $Z_1^{(1)} = 2$ and $Z_1^{(2)} = 1$ Eq. (51) describes XYZ models on ladders constituted by two coupled linear chains; the case $Z_1^{(1)} = 4$ and $Z_1^{(2)} = 1$ corresponds to models defined on two coupled square lattices. In both cases, every spin in each chain (plane), besides the usual interactions within a single chain (plane) involving $Z_1^{(1)}$ nearest neighbors, is also coupled to $Z_1^{(2)}$ companion spins located on the second chain (plane). The instance $Z_1^{(1)} = Z_1^{(2)} = 1$ corresponds to a XYZ-type model defined on a linear chain with nearest-neighbor interactions of alternating strengths. The factorization properties of this latter model have been studied by Giorgi³⁴ in the limit $f_z = g_z = 0$ that, belonging to the XY symmetry class, can be solved exactly.

As we have seen in Sec. IV, the first step of the method is to single out the magnetic order that minimizes the energy associated to the candidate factorized ground state, at fixed magnetization along the z direction (the direction of the external field). Provided there are no effects of frustration, in the present case we obtain that every possible hypothetical factorized ground state can assume one of eight different magnetic orders. These eight possibilities stem from the four possible orders of Eq. (13), that the system can support when the effects of g_α can be neglected, duplicated according to the two possible arrangements, parallel or antiparallel, induced by the interactions associated to g_α . The four possible orderings along a single direction are represented in Fig. 2 for a model of two transversally coupled one-dimensional spin chains.

By imposing the minimization of the energy per site, Eq. (10), the kind of order actually present in the ground state can be determined comparing the antiferromagnetic and ferromagnetic net interactions along the x and y axes, defined as

$$\mathcal{J}_\alpha^{\pm} = -Z_1^{(1)} f_\alpha \pm Z_1^{(2)} g_\alpha;$$

$$\mathcal{J}_\alpha^{\mp} = +Z_1^{(1)} f_\alpha \pm Z_1^{(2)} g_\alpha,$$

where the \pm sign discriminates between parallel/antiparallel ordering with respect to g_α . As a function of the net inter-

actions, the type of magnetic order present in the system is determined by the value of the minimum, i.e., of $\mu = \min\{\mathcal{J}_x^{F^+}, \mathcal{J}_x^{F^-}, \mathcal{J}_x^{A^+}, \mathcal{J}_x^{A^-}, \mathcal{J}_y^{F^+}, \mathcal{J}_y^{F^-}, \mathcal{J}_y^{A^+}, \mathcal{J}_y^{A^-}\}$. Accordingly, we have the following correspondences:

$$\mu = \begin{cases} \mathcal{J}_x^{F^+} \Rightarrow \text{Parallel ferromagnetic order along } x; \\ \mathcal{J}_x^{F^-} \Rightarrow \text{Antiparallel ferrom. order along } x; \\ \mathcal{J}_y^{F^+} \Rightarrow \text{Parallel ferrom. order along } y; \\ \mathcal{J}_y^{F^-} \Rightarrow \text{Antip. ferrom. order along } y; \\ \mathcal{J}_x^{A^+} \Rightarrow \text{Parallel antiferrom. order along } x; \\ \mathcal{J}_x^{A^-} \Rightarrow \text{Antip. antiferrom. order along } x; \\ \mathcal{J}_y^{A^+} \Rightarrow \text{Parallel antiferrom. order along } y; \\ \mathcal{J}_y^{A^-} \Rightarrow \text{Antip. antiferrom. order along } y. \end{cases} \quad (52)$$

Obviously, also in the presence of spatial anisotropies we may observe that, in terms of the net interactions, the fact that in the system there is no frustration (and especially no frustration arising from the spatial anisotropies) implies that $\mu = -Z_1^{(1)}|f_\alpha| - Z_1^{(2)}|g_\alpha|$, where $\alpha = x, y$ according to which axis is characterized by the given magnetic order.

Without loss of generality, let us consider the situation in which the system realizes a parallel antiferromagnetic order along the x direction, see Fig. 2(c). All other cases can be treated analogously. Following once again the steps described in Sec. IV, and in complete analogy with Eq. (28), it is possible to derive the set of conditions that the orientation θ of the E-SQUO must satisfy simultaneously in order for the system to admit a factorized energy eigenstate

$$\cos^2 \theta = \frac{f_y + f_z}{f_x + f_z} \quad (53)$$

$$\cos^2 \theta = \frac{g_y - g_z}{g_x - g_z}. \quad (54)$$

For the two conditions to be satisfied simultaneously the two rhs must coincide and must assume values in the interval $[0, 1]$. Hence, by equating them it is possible to derive an equation that plays the same role in Eqs. (43)–(46). In the hypothesis that the model under investigation satisfies both Eqs. (53) and (54), what is left to prove is that the associated factorized state be indeed the ground state. Following the route illustrated in Sec. IV it is not difficult to verify that the following inequalities must hold:

$$(f_x + f_y)(f_x + f_z) \geq 0; \quad f_x \geq -f_z; \quad (55)$$

$$(g_x + g_y)(g_x - g_z) \geq 0; \quad g_x \leq g_z. \quad (56)$$

It is straightforward to establish that they are both satisfied, provided there are no frustration effects. Namely, for spins interacting via couplings of the first kind f_α (referring to Fig. 2, these are the intrachain interactions), the second of Eq. (55) yields that the denominator in the rhs of Eq. (53) is non-negative and, therefore, the corresponding numerator

must be non-negative and not exceeding the denominator. Hence, we obtain $f_x \geq f_y$. On the other hand, from the first of Eq. (55) it follows that $f_x \geq -f_y$ which, in turn, implies $f_x \geq |f_y|$. The latter relation is in agreement with the hypothesis of absence of frustration. Furthermore, for pairs of neighboring spins interacting with a coupling of the second kind g_α (referring to Fig. 2, these are the interchain interactions), the second of Eq. (56) yields that the denominator in the rhs of Eq. (54) must be nonpositive. Hence, also the corresponding numerator must be nonpositive and therefore $g_x \leq g_y$. Simultaneously, the first of Eq. (56) implies $g_x \leq -g_y$ and therefore $g_x \leq |g_y|$, again in complete agreement with the hypothesis of absence of frustration. Collecting all these results we can conclude that in the absence of frustration, if a system described by the model Hamiltonian (51) satisfies simultaneously all conditions in Eqs. (53) and (54), there exist a factorizing field h_f at which the ground state is fully factorized and characterized by a parallel antiferromagnetic order along x . The factorizing field is determined according to the procedure described in Sec. IV, and it is not difficult to verify that it reads

$$h_f = \frac{1}{2} \sqrt{(\mathcal{J}_x^{A^+} - \mathcal{J}_z^{F^+})(\mathcal{J}_y^{A^+} - \mathcal{J}_z^{F^+})}. \quad (57)$$

The exact form of the factorized ground state reads

$$|\Psi_f\rangle = \otimes_k |\psi_k\rangle, \quad (58)$$

$$|\psi_k\rangle = (\cos(\theta/2)|\uparrow_k^u\rangle + e^{i\varphi_k} \sin(\theta/2)|\downarrow_k^u\rangle) \otimes (\cos(\theta/2)|\uparrow_k^l\rangle + e^{i\varphi_k} \sin(\theta/2)|\downarrow_k^l\rangle). \quad (59)$$

In Eq. (58), the superscript “ u ” (“ l ”) denotes the upper (lower) chain of the ladder model considered in Fig. 2(c). We observe that $\varphi_k = |k|\pi$ does not depend on the choice of the chain, implying that the two generic k th spins in both legs of the ladder are in the same state equipped with an antiferromagnetic order with respect to the nearest-neighbor sites along the corresponding chain. Analogous results hold, with the appropriate trivial modifications, when considering the other possible magnetic orders compatible with factorization [see Eq. (52)].

IX. CONCLUSIONS AND OUTLOOK

The present work has been motivated both by the need for exact solutions to complex many-body quantum spin models, in particular, by the question “when is a mean-field solution exact?” and by the necessity to acquire improved knowledge and control on the structure of quantum correlations for potential technological applications of spin systems. We have presented a simple and rather powerful all-analytic general method to determine the conditions for the existence and the properties of fully factorized (fully separable) ground states in translationally invariant quantum spin models with general two-body exchange interactions and subject to external fields.

The theory developed in the present paper builds on and extends the scheme originally introduced in Ref. 27. It pro-

vides a readily useful procedure to establish, in terms of the Hamiltonian parameters, whether the ground state is entangled or completely factorized and, in the latter case, what is the exact form of the state, the expression of the ground state energy and of the magnetic observables, and the type of ordered phase (magnetic order) compatible with factorization. The task is achieved by exploiting tools imported from quantum information theory such as the formalism of single-qubit unitary operations introduced in Refs. 28 and 29 and the corresponding entanglement excitation energies, whose property of vanishing, if and only if a quantum ground state is totally factorized, plays a central role in the analysis of ground state separability. Using these tools we have completed the program initiated in Ref. 27 by determining a general set of exact relations and inequalities that, for frustration-free systems, allow to establish rigorously the occurrence of all types of possible factorized ground states.

We have applied the analytic method to spin-1/2 models with general Heisenberg-type exchange interactions of arbitrary range (short, finite, and long), either isotropic or anisotropic, defined on regular lattices of arbitrary dimensions. The method is insensitive to the size of the system and applies rigorously in the thermodynamic limit as well as for finite lattices. The method allows to establish exact, fully factorized ground state solutions of generally nonexactly solvable models, corresponding to nontrivial sets of values of the Hamiltonian parameters. Key results include, for instance, the rather straightforward determination of the existence and form of factorized ground states in XYZ-type models with different types of short-range and long-range interactions on cubic lattices, a task that would be of formidable complexity if tackled with numerical techniques or resorting to the simple-minded direct method based on the product ansatz.

The complete factorization diagram for nearest-neighbor Heisenberg-type anisotropic models might be particularly useful for those technological implementations which employ spin systems as information processors exploiting their ground state entanglement.¹⁴ We have provided in Fig. 1(a) “minefield” map of the unentangled working points that need to be avoided, when engineering the couplings and tuning the external fields, in order to achieve satisfactory quantum transmission performances. On the other hand, there are also alternative tasks in quantum information which instead require as initial working points factorized states, e.g., for engineering, via suitable dynamics, specific classes of long-distance entangled states useful for quantum state transfer and quantum teleportation⁴¹ or the instantaneous creation of strongly entangled graphs or cluster states involving a mesoscopic or macroscopic number of spins for one-way quantum computation:⁴² in these instances the minefield may turn into a treasure map. The analysis of ground state factorization would be particularly useful in the study of quantum spin models on open-end lattices. Such systems are not translationally invariant, and therefore the analytic method requires to be suitably extended to this type of instances. This generalization is under way and should be in reach in the near future.

Notably, according to a general theorem by Kurmann *et al.*²⁰ on factorization, given any Hamiltonian of the form Eq.

(6) involving higher spins $S > 1/2$, the ground state of that spin- S system is fully factorized at the same value of the external field $h = h_f$ Eq. (30), at which factorization occurs in the corresponding spin-1/2 model. Therefore, the method and the results derived in the present paper have a much wider scope of application and can be straightforwardly generalized to interacting systems with arbitrarily high values of the spin, provided they are of the same Hamiltonian structure as in the spin-1/2 case.

Absence of frustration effects, either of geometric or dynamical nature, has been essential to the theoretical scheme derived in the present work. For instance, we have determined the factorization diagram for specific examples of frustration-free systems endowed with isotropic interaction terms of different spatial ranges, and for systems with nearest-neighbor anisotropic interactions. However, it is clear that there are many extremely interesting instances of more complex systems that would in general be subject to frustration effects. Continuing a step-by-step strategy of applying the general method to models of increasing complexity, natural further stages of investigation would include models subject to frustration, e.g., models on linear chains with competing isotropic interactions of different range such as a 1D XYZ-type model with nearest-neighbor ferromagnetic interactions and next-to-nearest-neighbor antiferromagnetic interactions. Increasing further the degree of complexity, one could then consider models with competing anisotropic interactions of different ranges, that according to the type of anisotropy could be subject to both geometrically and dynamically induced frustrations.

When considering frustrated models, except for very special cases, even when the considered system admits a fully factorized state as an energy eigenstate, the set of conditions derived in the present work are not sufficient to establish that such an eigenstate is indeed the ground state of the system. In fact, a competition arises between factorization, which requires a magnetic ordering, and frustration, which tends to destroy magnetic orders, ultimately leading to a chaotic correlating behavior. The latter unavoidably tends to enhance ground state entanglement, thus suppressing the occurrence of situations where the most favorable state, in terms of energy content, is completely uncorrelated. In such cases, a naive application of the direct method based on the factorized ansatz, for instance, to models including anisotropic interaction terms of different magnetic types on many different spatial scales (or even on all scales), leads unavoidably to overestimate the factorizing effect of the balancing between interactions and external fields and thus to badly incorrect predictions on the occurrence of fully factorized ground states in these classes of models, as done, unfortunately, in the second part of Ref. 34. In a forthcoming work³⁶ we will present a systematic and thorough study of some important classes of frustrated quantum spin models in order to establish the conditions for the occurrence of true ground state factorization and to characterize it in terms of compatibility thresholds with frustration.

An intriguing issue that arises in connection with frustration is the relationship between factorization and the existence of ordered phases. For frustration-free Hamiltonian systems that conserve the even-odd parity, spontaneous sym-

metry breaking, and the existence of an ordered phase are necessary conditions for ground state factorization, because factorized states have no definite parity. However, in the presence of frustration there may exist factorized energy eigenstates without ground state factorization. It would then be very interesting to understand whether in these situations there is still a causal relation between factorization and the existence of phase transitions in the system. Factorization might then be used as an heuristic tool to gain insight in the phase diagram of frustrated quantum systems.

It would also be important to understand whether chiral interactions can enhance factorization beyond the limits imposed by the presence of frustration effects. In fact, since factorization can be seen as “mean field becoming exact,” it seems to require quite naturally a balancing between interactions and external fields as the only possibility for its occurrence. However, one cannot exclude, in principle, that other mechanisms might lead to the same effect without requiring the presence of external driving fields.

Future investigations will be concerned with the application of the analytic method to the determination of the spectrum of factorization, that is the study of the occurrence of factorized excited states in different classes of quantum spin Hamiltonians, and the implications of factorization diagrams on the structural and informational properties of quantum spin models for potential applications in quantum technology.

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APPENDIX: DETERMINATION OF THE MAGNETIC ORDERINGS COMPATIBLE WITH GROUND STATE FACTORIZATION

In Sec. IV we have determined the general conditions for ground state factorization by selecting as candidate factorized ground states only those characterized by a ferromagnetic or antiferromagnetic order along the x or y direction depending on the value of the minimum value μ in the set of the net interactions [see Eq. (13)], and neglecting all other possible magnetic arrangements. In the following, we will prove that indeed, given any spin Hamiltonian of the type Eq. (6), if a factorized ground state exists, then it is characterized by one of the four above-mentioned magnetic orders.

Let us consider the most general factorized state compatible with the constraint of a site-independent magnetization M_z

$$|\Psi_f\rangle = \otimes_k |\psi_k\rangle, \quad |\psi_k\rangle = \cos(\theta/2)|\uparrow_k\rangle + e^{i\varphi_k} \sin(\theta/2)|\downarrow_k\rangle,$$

where the local spin state $|\psi_k\rangle$ is eigenstate of

$$\bar{O}_k = \cos \theta S_k^z + \cos \varphi_k \sin \theta S_k^x + \sin \varphi_k \sin \theta S_k^y, \quad (\text{A1})$$

with eigenvalue equal to 1/2. Let us suppose that there exists a Hamiltonian of the type Eq. (6) that admits, for some par-

ticular value of the external field $h=h_f$, the state in Eq. (A1) as an eigenstate. Under these hypotheses we must have that the projection of the factorized eigenstate onto the four-dimensional Hilbert space of a pair of spins in the lattice must be an eigenstate of the pair-Hamiltonian term $H_{\underline{i}\underline{j}}$ defined as in Eq. (23).

Following the same strategy as in Sec. IV let us introduce for each site \underline{i} a set of three auxiliary mutually orthogonal spin operators among which one, that we name $A_{\underline{i}}^z$, coincides with $\bar{O}_{\underline{i}}$

$$\begin{aligned} A_{\underline{i}}^x &= \cos \theta \cos \varphi_{\underline{i}} S_{\underline{i}}^x + \cos \theta \sin \varphi_{\underline{i}} S_{\underline{i}}^y - \sin \theta S_{\underline{i}}^z; \\ A_{\underline{i}}^y &= -\sin \varphi_{\underline{i}} S_{\underline{i}}^x + \cos \varphi_{\underline{i}} S_{\underline{i}}^y; \\ A_{\underline{i}}^z &= \sin \theta \cos \varphi_{\underline{i}} S_{\underline{i}}^x + \sin \theta \sin \varphi_{\underline{i}} S_{\underline{i}}^y + \cos \theta S_{\underline{i}}^z. \end{aligned} \quad (\text{A2})$$

By inverting Eqs. (A2), we can conveniently re-express the conventional single-spin operators as functions of the new set of operators $\{A_{\underline{i}}^\alpha\}$

$$\begin{aligned} S_{\underline{i}}^x &= A_{\underline{i}}^x \cos \theta \cos \varphi_{\underline{i}} - A_{\underline{i}}^y \sin \varphi_{\underline{i}} + A_{\underline{i}}^z \sin \theta \cos \varphi_{\underline{i}}; \\ S_{\underline{i}}^y &= A_{\underline{i}}^x \cos \theta \sin \varphi_{\underline{i}} + A_{\underline{i}}^y \cos \varphi_{\underline{i}} + A_{\underline{i}}^z \sin \theta \sin \varphi_{\underline{i}}; \\ S_{\underline{i}}^z &= -A_{\underline{i}}^x \sin \theta + A_{\underline{i}}^z \cos \theta. \end{aligned} \quad (\text{A3})$$

Substituting Eq. (A3) into the pair Hamiltonian we obtain the expression for $H_{\underline{i}\underline{j}}$ at factorization as a function of the sets of operators $\{A_{\underline{i}}^\alpha\}$ and $\{A_{\underline{j}}^\alpha\}$, which reads

$$\begin{aligned} H_{\underline{i}\underline{j}} &= A_{\underline{i}}^z A_{\underline{j}}^z [\cos^2 \theta J_z^r + \sin^2 \theta (J_x^r \cos \varphi_{\underline{i}} \cos \varphi_{\underline{j}} \\ &\quad + J_y^r \sin \varphi_{\underline{i}} \sin \varphi_{\underline{j}})] - 2h_f^r \sin \theta \left[A_{\underline{i}}^x \left(A_{\underline{j}}^z - \frac{1}{2} \right) \right. \\ &\quad \left. + \left(A_{\underline{i}}^z - \frac{1}{2} \right) A_{\underline{j}}^x \right] + A_{\underline{i}}^x A_{\underline{j}}^x (J_z^r - 2h_f^r \cos \theta) \\ &\quad + A_{\underline{i}}^y A_{\underline{j}}^y (J_x^r \sin \varphi_{\underline{i}} \sin \varphi_{\underline{j}} + J_y^r \cos \varphi_{\underline{i}} \cos \varphi_{\underline{j}}) \\ &\quad - h_f^r \cos \theta (A_{\underline{i}}^z + A_{\underline{j}}^z) + (A_{\underline{i}}^z A_{\underline{j}}^y \cos \theta + A_{\underline{i}}^x A_{\underline{j}}^y \sin \theta) \\ &\quad \times (-J_x^r \cos \varphi_{\underline{i}} \sin \varphi_{\underline{j}} + J_y^r \sin \varphi_{\underline{i}} \cos \varphi_{\underline{j}}) + (A_{\underline{i}}^y A_{\underline{j}}^z \cos \theta \\ &\quad + A_{\underline{i}}^y A_{\underline{j}}^x \sin \theta) (-J_x^r \sin \varphi_{\underline{i}} \cos \varphi_{\underline{j}} + J_y^r \cos \varphi_{\underline{i}} \sin \varphi_{\underline{j}}), \end{aligned} \quad (\text{A4})$$

where, as usual, r is the distance between sites \underline{i} and \underline{j} , J_α^r are the spin-spin couplings at distance r and along direction α , and

h_f^r obeys to the following relation

$$2h_f^r = \cos \theta (J_z^r - \cos \varphi_{\underline{i}} \cos \varphi_{\underline{j}} J_x^r - \sin \varphi_{\underline{i}} \sin \varphi_{\underline{j}} J_y^r). \quad (\text{A5})$$

From Eq. (A4), one has that to ensure that the projection of the factorized state onto the four-dimensional Hilbert space of spins S_i and S_j is an eigenstate of the pair Hamiltonian, it is necessary to require that the terms associated to the operators $A_i^x A_j^y$, $A_i^y A_j^x$, $A_i^z A_j^z$, and $A_j^y A_i^z$ vanish. This condition yields that

$$J_x^r \cos \varphi_i \sin \varphi_j = J_y^r \sin \varphi_i \cos \varphi_j, \quad (\text{A6})$$

$$J_x^r \sin \varphi_i \cos \varphi_j = J_y^r \cos \varphi_i \sin \varphi_j. \quad (\text{A7})$$

Solving Eqs. (A6) and (A7) we obtain that if $|J_x^r| \neq |J_y^r|$, then the phases φ obey to the following relations:

$$\varphi_i = 0, \pi/2 \quad \varphi_j = \varphi_i + n\pi, \quad (\text{A8})$$

with n integer. It is immediate to verify that these relations are consistent only with a ferromagnetic or with an antiferromagnetic order along the x or y direction. This concludes the proof.

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