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Factorized ground state for a general class of ferrimagnets

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We have found the exact (factorized) ground state of a general class of ferrimagnets in the presence of a magnetic field which includes the anisotropic and long-range interactions for arbitrary dimensional space. In particular cases our model represents many spin chains with bond alternation of antiferromagnetic-ferromagnetic coupling, ferrimagnetic spin ladders, and also homogeneous spin-*s* models. The factorized ground state is a product of single-particle kets on a bipartite lattice composed of two different spins (ρ,σ) which is characterized by two angles, a *biangle* state. The spin-wave analysis around the exact ground state shows two branch of excitations which are the origin of two dynamics of the model. The signature of these dynamics is addressed as a peak and a broaden bump in the specific heat.

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I. INTRODUCTION

Spin models are the building blocks of the theory of quantum magnetism and strongly correlated electron systems. In addition, they have been considered as an effective model to describe the behavior of a system in several disciplines. Recently, the implementation of quantum notions in quantum devices has attracted much attention both in research laboratories and demanding applications such as nanotechnology, quantum computation,[1] and particularly optical lattices.[2] Quantum spin models are prototype realization of many relevant properties of quantum implementation in such devices. Therefore, different aspects of a quantum phase are of utmost importance for scientists and engineers. Quantum phases are characterized by the ground-state (GS) properties of the corresponding many-body system.[3] The investigation to find the GS of a many-body model has been a major subject of the mentioned fields of research.

In the area of spin models, except of a few particular cases such as one-dimensional (1D) bond alternating Heisenberg spin-1/2 chains,[4] anisotropic Heisenberg (*XYZ*), *XXZ* model in a longitudinal magnetic field and Ising model in transverse field which are exactly solvable,[5] the GS of a general spin model is not known. However, at some particular values of the model parameters the quantum correlations are vanishing and the GS can be found exactly as a product of single-particle states. The existence and knowledge of an exact factorized state (FS) have several important features. (i) It manifests zero entanglement which is necessary to be identified for reliable manipulating of quantum computing. (ii) A FS which is associated with an entanglement phase transition can be also a quantum critical point in certain condition which is discussed in this Rapid Communication. This information is also attractive for the study of quantum phase transitions. (iii) Moreover, finding an exact ground state even at particular values of the parameter space of a many-body spin model leads to the identification of that phase in addition to more knowledge about the properties of the model close to the factorized point via implementing an approximate method.

In a seminal work, Kurmann *et al.*[6] identified the factorized state of a homogeneous spin-*s* *XYZ* chain at a magnetic field of arbitrary direction. Factorized GS has been also observed in the two-dimensional lattice through quantum Monte Carlo simulation in terms of entanglement estimators.[7] Recently, Giampaolo *et al.*[8,9] introduced a general analytic approach to find the factorized ground states in a homogenous *translational invariant* spin-*s* quantum spin model for arbitrary long-range interaction and any dimensional space. Their study is based on the single-spin unitary operation and the factorized point is determined at the position where the associated entanglement excitation energy becomes zero. The factorized GS of the dimerized *XYZ* spin chain in a transverse magnetic field has been investigated and reported that the factorized point in the parameter space of the Hamiltonian corresponds to an accidental ground-state degeneracy.[10] However, in this Rapid Communication we will present (i) the FS of an inhomogeneous (ferrimagnetic) spin model which is composed of two spins (ρ,σ) in the presence of a magnetic field on a bipartite lattice with arbitrary long-range interaction and dimensional space, (ii) the Hamiltonian is not necessarily translational invariant, and (iii) the exchange couplings can be competing antiferromagnetic and ferromagnetic arbitrarily between different sublattices to build many practical models such as frustrated, dimerized, and tetramerized materials. Moreover, our results recover the previous ones for $\sigma=\rho$ and a particular configuration of the couplings.[6–8,10] In addition, we will address on the existence of two energy scales which lead to a surprising dynamics of the model close to the factorizing point and its fingerprint as a double peak in the specific heat versus temperature. As an enclosure, the results have been applied to the 1D ferrimagnetic *XXZ* (ρ,σ) spin chain in the presence of a transverse magnetic field which is realized as a bimetallic substance.[11] We will also address the cases where the factorizing field coincides the critical point.

II. FACTORIZED STATE

Let us consider a two sites model which is composed of two spins $\sigma=\frac{1}{2}$ and $\rho=1$ with the following Hamiltonian:

$$H' = J^x\sigma^x\rho^x + J^y\sigma^y\rho^y + J^z\sigma^z\rho^z + h'(\sigma_z+\rho_z), \quad (1)$$

where J^μ, $\mu=x,y,z$, are the exchange couplings in different directions and h' is proportional to the magnetic field. We are looking for a factorized state which is satisfied by $H'|\sigma\rangle|\rho\rangle = \epsilon|\sigma\rangle|\rho\rangle$, in which $|\sigma\rangle$ and $|\rho\rangle$ are the single-particle states. It is appropriate to choose $|\sigma\rangle$ and $|\rho\rangle$ to be the eigenstates of $\vec{\sigma}\cdot\hat{n}'$ and $\vec{\rho}\cdot\hat{n}''$ with eigenvalues $+\frac{1}{2}$ and $+1$; respectively, where $\hat{n}'(\theta,\varphi)$ and $\hat{n}''(\beta,\alpha)$ are unit vectors in Bloch sphere. The solution of $H'|\sigma\rangle|\rho\rangle=\epsilon|\sigma\rangle|\rho\rangle$ gives the factorized state at $h'=h'_f$ and its corresponding energy (ϵ).[12] Moreover, we found that the angles θ and β are fixed by the couplings [J^μ,h'; see Eq. (2)], while α and φ are given by one of these choices (I) $\alpha=0$ and $\varphi=0$; (II) $\alpha=0$ and $\varphi=\pi$; (III) $\alpha=\frac{\pi}{2}$ and $\varphi=-\frac{\pi}{2}$; and (IV) $\alpha=\frac{\pi}{2}$ and $\varphi=\frac{\pi}{2}$. The spins are located in the xz plane for choices I and II while they have projections only in the yz plane for III and IV. Without loss of generality we can assume the spins are located in the xz plane. In fact, the spins of yz plane will fall to xz plane by interchange of $J^x\leftrightarrow J^y$. Moreover, the coordinates $(\theta,\varphi=0)$ and $(-\theta,\varphi=\pi)$ are representing the same direction, therefore case (I) $\alpha=0$, $\varphi=0$ is able to describe all possibilities.

The two spin model $(\sigma=\frac{1}{2},\rho=1)$ is now generalized to arbitrary (σ,ρ) spins.[6] To find the factorized state of a general two site ferrimagnet we consider a rotation on σ and ρ spins such that $\vec{\sigma}$ and $\vec{\rho}$ point in $(\theta,\varphi=0)$ and $(\beta,\alpha=0)$ directions, respectively, The rotation operator is $D=D^\sigma(0,\theta,0)D^\rho(0,\beta,0)$ where $D^\rho(0,\beta,0)=D(\alpha=0,\beta,\gamma=0)=D_z(\alpha)D_y(\beta)D_z(\gamma)$ is defined in terms of Euler angles and a similar expression is considered for $D^\sigma(0,\theta,0)$. Then, we impose the condition to have a factorized (fully polarized) eigenstate for this Hamiltonian which fixes the following relations for the model parameters:

$$\cos\theta = -\frac{h_f'^2J^y + J^x(J^{z^2}-J^{y^2})\rho\sigma + h_f'J^z(J^y\rho+J^x\sigma)}{h_f'^2J^x + J^y(J^{z^2}-J^{x^2})\rho\sigma + h_f'J^z(J^x\rho+J^y\sigma)},$$

$$\cos\beta = -\frac{h_f'^2J^y + J^x(J^{z^2}-J^{y^2})\rho\sigma + h_f'J^z(J^y\sigma+J^x\rho)}{h_f'^2J^x + J^y(J^{z^2}-J^{x^2})\rho\sigma + h_f'J^z(J^x\sigma+J^y\rho)},$$

$$h_f' = \sqrt{\tfrac{1}{2}(2J^xJ^y\rho\sigma + (\rho^2+\sigma^2)J^{z^2} + CJ^z)},$$

$$C \equiv \sqrt{4\rho\sigma(\rho J^x+\sigma J^y)(\sigma J^x+\rho J^y) + (\rho^2-\sigma^2)^2J^{z^2}},$$

$$\epsilon = \frac{J^xJ^y}{J^z}\sigma\rho - \frac{h_f'^2}{J^z}. \quad (2)$$

Therefore, for arbitrary (σ,ρ) and at the above value for $h'=h'_f$ we have a fully polarized eigenstate which is a factorized state. The ordering of this state is defined by two angles (θ,β) which show the orientations of $(\vec{\sigma},\vec{\rho})$, respectively.

Now, we intend to find the condition for having a factorized state for a ferrimagnetic lattice in a magnetic field. We consider a general Hamiltonian of ferrimagnets on a bipartite lattice where sublattice (A_σ) contains σ spins and the other sublattice (B_ρ) includes ρ spins. The interaction can be long ranged between different sublattices but no interaction in the same sublattice. The ferrimagnetic Hamiltonian for such case can be written as

$$H = \sum_{i,r}[\zeta_i\hat{\zeta}_{i+r}(J_r^x\sigma_i^x\rho_{i+r}^x + J_r^y\sigma_i^y\rho_{i+r}^y) + J_r^z\sigma_i^z\rho_{i+r}^z] + h\sum_i(\sigma_i^z+\rho_i^z), \quad (3)$$

where $i=(i_1,i_2,i_3)$ and $r=(r_1,r_2,r_3)$ are representing the three dimensional index on the lattice and ζ_i, $\hat{\zeta}_{i+r}=\pm1$ which realize both ferromagnetic (F) and antiferromagnetic (AF) exchange interactions. A remark is in order here, the Hamiltonian in Eq. (3) is a sum of two sites Hamiltonian defined in Eq. (1) where the two spins can be far from each other. However, the interaction between each couple of (σ_i,ρ_{i+r}) can depend on distance (r) with different strength and also be F or AF arbitrarily defined by ζ_i and $\hat{\zeta}_{i+r}$. A factorized eigenstate for the Hamiltonian of Eq. (3) can be written as

$$|\mathrm{FS}\rangle = \bigotimes_{i\in A_\sigma, j\in B_\rho}|\sigma_i'\rangle|\rho_j''\rangle, \quad (4)$$

where $|\sigma_i'\rangle$ and $|\rho_j''\rangle$ are the eigenstates of $\vec{\sigma}_i\cdot\hat{n}_i'$ and $\vec{\rho}_j\cdot\hat{n}_j''$ with largest eigenvalue where $\hat{n}_i'$ and $\hat{n}_j''$ are unit vectors pointing in $(\zeta_i\theta,\varphi=0)$ and $(\hat{\zeta}_j\beta,\alpha=0)$, respectively. However, the factorized state ($|\mathrm{FS}\rangle$) is an eigenstate of the Hamiltonian if the angle $\zeta_i\theta(\hat{\zeta}_j\beta)$ be consistent with all pair of interactions originating from $\sigma_i(\rho_i)$ on sublattices $A_\sigma(B_\rho)$. According to Eq. (2) the former condition is satisfied if the interaction between each pair (σ_i,ρ_{i+r}) is the same for all directions while depending on distance (r), i.e., $J_r^\mu=\lambda(r)J^\mu$, $\mu=x,y,z$, and $\lambda(r)>0$. Under these constraints the factorized state [Eq. (4)] is an eigenstate of H with the characteristic angles (θ,β) defined in Eq. (2) and the factorizing field is

$$h_f = h_f'\sum_{r=0}^{N_r}\lambda(r), \quad (5)$$

where N_r is the number of spins on each sublattice.

To show that $|\mathrm{FS}\rangle$ is the ground state of H at h_f, let us first consider the case of $(\sigma=1/2,\rho=1)$. The two spin Hamiltonian (1) is diagonalized exactly at h'_f defined in Eq. (2). The ground-state energy is found to be ϵ if $J^z>\mathrm{sgn}(-J^xJ^y)\times\min\{|J^x|,|J^y|\}$. And the corresponding factorized eigenstate is defined by θ and β which are given by Eq. (2). Moreover, the many-body Hamiltonian (H) defined in Eq. (3) can be written as sum of two spin parts, i.e., $H=\sum_{i,j}H'_{i,j}$. The Hamiltonian can be expressed as $H-N_b\epsilon=\sum_{i,j}(H'_{i,j}-\epsilon)$ which is a sum of positive definite terms where N_b is the number of interacting spin pairs (i,j). It is now clear that $(H-N_b\epsilon)|\mathrm{FS}\rangle=0$ which verifies that $|\mathrm{FS}\rangle$ is the ground state of H. A similar calculation for $(\sigma=1,\rho=2)$ gives the same condition $J^z>\mathrm{sgn}(-J^xJ^y)\times\min\{|J^x|,|J^y|\}$ such that $|\mathrm{FS}\rangle$ be the ground state. The exact diagonalization of arbitrary (σ,ρ) pair is not known, especially for large values of spins. However, the condition mentioned above is independent of the spin magnitude which leads us to conclude that it will be the case for arbitrary (σ,ρ) case.

To justify our claim we implement a linear spin-wave approximation. We first implement a rotation on the Hamiltonian. The rotated Hamiltonian $(\widetilde{H})$ is the result of rotations on all lattice points of H, $\widetilde{H}=\widetilde{D}^{\dagger}H\widetilde{D}$, and $\widetilde{D}=\otimes_{i\in A_{\sigma},j\in B_{\rho}}D_i^{\sigma}(0,\zeta_i\theta,0)D_j^{\rho}(0,\hat{\zeta}_j\beta,0)$. In the next step the rotated Hamiltonian is bosonized using the Holstein-Primakoff (HP) transformation, $\sigma_i^{+}=\sqrt{2\sigma-a_i^{\dagger}a_i}a_i$, $\sigma_i^{z'}=\sigma-a_i^{\dagger}a_i$, $\rho_j^{+}=\sqrt{2\rho-b_j^{\dagger}b_j}b_j$, and $\rho_j^{z''}=\rho-b_j^{\dagger}b_j$ where $a_i(a_i^{\dagger})$ and $b_j(b_j^{\dagger})$ are two types annihilation (creation) boson operators. The Hamiltonian in the momentum (k) space and in the linear spin-wave theory (LSWT) is diagonalized via the rotation, $\chi_k=a_k\cos\eta_k-e^{i\delta}b_k\sin\eta_k$; $\psi_k=e^{i\delta}b_k\cos\eta_k+a_k\sin\eta_k$, and a shift at $k=0$ where δ is defined by $\Sigma_r e^{-ik\cdot r}J_r^{y}=|\Sigma_r e^{-ik\cdot r}J_r^{y}|e^{i\delta}$. The diagonalized Hamiltonian is

$$\widetilde{H}=E_{gs}+\sum_k(\omega^{-}(k)\chi_k^{\dagger}\chi_k+\omega^{+}(k)\psi_k^{\dagger}\psi_k), \quad (6)$$

where E_{gs} is the ground-state energy[12] and $\omega^{\pm}(k)\geq 0$ are normal modes parallel and perpendicular to the field direction. The energy modes are positive as far as $J^z>\text{sgn}(-J^xJ^y)\times\min\{|J^x|,|J^y|\}$.

$$\omega^{\pm}(k)=D^{+}\pm\frac{D^{-}+\sqrt{\sigma\rho}\tan(2\eta_k)|\Sigma_r e^{-ik\cdot r}J_r^{y}|}{\sqrt{1+\tan^2(2\eta_k)}},$$

$$\tan(2\eta_k)=\frac{\sqrt{\rho\sigma}|\Sigma_r e^{-ik\cdot r}J_r^{y}|}{D^{-}}, \quad (7)$$

in which

$$D^{\pm}\equiv\frac{h_f^2}{2\tau^z}\left(\frac{1}{\rho}\pm\frac{1}{\sigma}\right)+h_f\left(\frac{\sigma}{2\rho}\cos\theta\pm\frac{\rho}{2\sigma}\cos\beta\right)-\frac{\tau^x\tau^y}{2\tau^z}(\sigma\pm\rho)+\frac{h_f-h}{2}(\cos\beta\pm\cos\theta), \quad (8)$$

where $\tau^{\mu}=J^{\mu}\Sigma_r\lambda(r)$. The bosonized Hamiltonian (6) is positive definite, $(\omega^{\pm}(k)\geq 0)$, which states that $|\text{FS}\rangle$ is its corresponding ground state. Although the excitation spectrum of the LSWT is not exact generally it has been shown[13] that the LSWT spectrum is exact at the ordering wave vector for a homogenous Heisenberg spin model. It is then anticipated that in our case the spectrum being exact at $k=0$ which represents the minimum excitation energy. Thus, the condition for $\omega^{\pm}(k=0)>0$ makes $\widetilde{H}-E_{gs}$ be positive definite. This condition is again the same as what we obtained for the special cases of $(\sigma=1/2,\rho=1)$ and $(\sigma=1,\rho=2)$, i.e., $J^z>\text{sgn}(-J^xJ^y)\times\min\{|J^x|,|J^y|\}$.

To visualize the configuration of a factorized ground state of a general interacting model, we have plotted an example in Fig. 1 with the assumption J_r^x, $J_r^y>0$ and $J_r^z<0$, where ζ_i and $\hat{\zeta}_{i+r}$ define the sign of interactions. The solid lines represent antiferromagnetic interaction and the dash-dotted ones are the ferromagnetic counterparts. As shown in Fig. 1 the interactions can be long ranged without a translational invariance. However, the factorized state is defined by two angles (θ,β) while each $\sigma(\rho)$ spin is directed in $\theta(\beta)$ or $-\theta(-\beta)$ directions. We call this a *biangle* ordering. In a special case the biangle ordered state can configure a ferromagnet $(\theta=\beta)$ or antiferromagnet $(\theta=-\beta)$ factorized state.

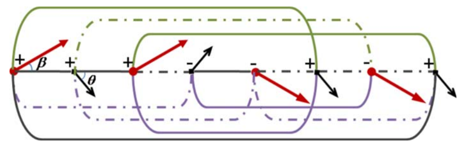

FIG. 1. (Color online) The configuration of a factorized state on a one-dimensional lattice for arbitrary frustration-free combinations of the couplings. Solid lines (dash-dotted) represent antiferromagnetic (ferromagnetic) couplings which are defined by $\zeta_i\hat{\zeta}_{i+r}$ as depicted by $\pm$ on each site. Each color belongs to equal distance interaction (same r).

III. DISCUSSIONS

In a spin model when the magnetic field is strong enough all spins will align in the direction of the magnetic field which characterizes the saturated phase as far as $h\geq h_s$. In our notation, the saturated phase appears when all $\sigma(\rho)$ spins get $\theta=\pi(\beta=\pi)$. Thus, the saturating field (h_s) is a factorizing one when $J^x=J^y$. In case of $J^x\neq J^y$ the saturation can only appear at infinite value of the magnetic field while a finite factorizing point (h_f) still exists. For $J^x=J^y$, the lower excitation band becomes gapless $[\omega^{-}(k=0)=0]$ which confirms that the factorizing point $(h_f=h_s)$ is the critical point which separates the non-saturated phase $(h<h_s)$ from the saturated one $(h>h_s)$. It is worth to mention that at $J^x=J^y$ the rotational symmetry around the magnetic field is restored where the quantum fluctuations around the field axis are suppressed.

A general feature of our result is that it can simply recover the previous study of homogenous systems by replacing $\sigma=\rho=s$. In that case the restriction of bipartite lattice is promoted to arbitrary lattice and the interaction between any pair of spins can exist. In the presence of frustration, the normal modes in Eq. (6) are not always positive definite. This constraint thus limits the set of admissible coupling constants.[12] However, our Hamiltonian is not restricted to the translational invariant symmetry or bond-alternating ones which is witnessed by the example given in Fig. 1. This can also be generalized to any dimension. We claim that the general Hamiltonian which can possess a nontrivial factorized ground state should be of the form Eq. (3) with the restriction $J_r^{\mu}=\lambda(r)J^{\mu}$, $\mu=x,y,z$.

Let us now be more concrete by concentrating on the one-dimensional nearest-neighbor $(\sigma=1/2,\rho=1)$ *XXZ* ferrimagnet in the presence of transverse magnetic field. Suppose that $J^x=J^z=J$ and $J^y=J\Delta$, where Δ represents the easy axis anisotropy. At zero magnetic field the quantum fluctuations are large and the ground state of the model is strongly entangled. Upon adding the transverse magnetic field the U(1) symmetry of the *XXZ* model is lost and the entanglement of the GS is decreased. In the mapped bosonic system the magnetic field is served as a chemical potential, thus the number of bosons ($\langle a^{\dagger}a\rangle$ and $\langle b^{\dagger}b\rangle$) is dependent on the magnetic field. An enchantment of the magnetic field causes deducing of the bosons' number and the quantum correlations decrease. At factorizing field $h=h_f$, the number of bosons is zero and the quantum fluctuations become completely uncorrelated. Moreover, our calculations show that the factorizing field in ferrimagnetic model depends on the anisotropy parameter (Δ) similar to a homogeneous antiferromagnetic Heisenberg model. Increasing Δ from zero suppresses the effect of magnetic field and try to evoke the rotational symmetry to the system. Thus, by increasing Δ the factorizing field approaches to the saturation field. At $\Delta=1$, the rotational symmetry is completely repayed and h_f is exactly lied on h_s.

A benefit of identification a factorized state is that we can work out an approximate method around the factorized point to get some information on the properties of that phase. This helps us to calculate the magnetic properties of the ferrimagnetic *XXZ* model in the presence of a transverse magnetic field. We have implemented the linear spin-wave theory around $h=h_f$ for $\sigma=\frac{1}{2}$ and $\rho=1$. Our results for magnetization (M_x,M_y) and staggered magnetization (SM_x,SM_y) in both x and y directions are plotted in Fig. 2 where the magnetic field is in x direction.

It is also worth to mention that our results are applicable to the homogenous *XXZ* Heisenberg spin-1/2 chains in the presence of a transverse magnetic field (h^x). This model has been studied intensively in the literature.[14–17] The excitation energies around the factorizing field are $\omega^{\pm}(k)=(1+\Delta)\frac{h}{h_f}+\Delta[\pm\cos(\frac{k}{2})-1]$. Thus, we have two branches of magnon energies as two scales of energy which impose two dynamics in the system. The most interesting feature is that around the factorizing field both scales show up. These dynamics correspond to the coexistence of two different features of the model. The finger print of these features appear in the thermodynamic functions such as specific heat and internal energy. As it is seen from Ref. 17 the second feature can be seen as a shoulder at the right side of specific-heat curve. By further increasing of h, the ferromagnetic behavior is seen as a broaden peak in the curve. This point is almost near the classical field where the ground state of the system has been factorized.

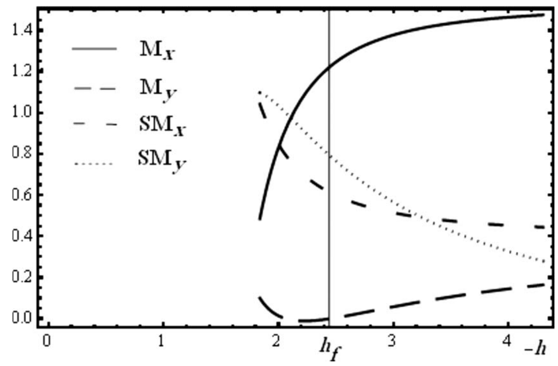

FIG. 2. The magnetization and staggered magnetization of an anisotropic ferrimagnetic ($\sigma=1/2,\rho=1$) spin chain versus transverse field and for $\Delta=0.25$.

Note added. Recently, a preprint on the factorized state of the frustrated homogenous spin model appeared.[18] It has been shown that the factorized state which has been defined in Eq. (4) is the ground state of the whole system as far as the frustration strength is weak, while for strong frustration it will be an excited state.

ACKNOWLEDGMENTS

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