Exact Ground States of a Frustrated 2D Magnet: Deconfined Fractional Excitations at a First-Order Quantum Phase Transition

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We introduce a frustrated spin 1/2 Hamiltonian which is an extension of the two dimensional $J_1 - J_2$ Heisenberg model. The ground states of this model are exactly obtained at a first-order quantum phase transition between two valence bond crystals. At this point, the low energy excitations are deconfined spinons and spin-charge separation occurs under doping in the limit of low concentration of holes. In addition, this point is characterized by the proliferation of topological defects.

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Frustrated magnets are the focus of considerable attention because exotic quantum effects are expected to emerge from the competition between opposite tendencies. While several models in this category are solvable in one dimension, the list is much smaller for higher dimensions. One of the most studied frustrated magnets is the spin 1/2 Heisenberg model with first and second nearest neighbor interactions J_1 and J_2. In one dimension, this model exhibits a quantum transition as a function of J_2/J_1 from a critical state with quasi-long-range antiferromagnetic (AF) order to a dimerized phase. In contrast, two dimensional (2D) frustrated magnets such as the $J_1 - J_2$ Heisenberg model on a square lattice still hold many secrets. Different approaches predict a transition between a Néel ordered state and a gapped (nonmagnetic) quantum phase for the region $0.4 \lesssim J_2/J_1 \lesssim 0.6$. However, the nature of this phase is still debated. More precisely, the question is whether it is a uniform spin liquid [1] or a spatially ordered valence bond crystal (VBC) [2].

The interest in frustration and magnetism is not limited to this widely debated question. There are reasons to believe that frustrated magnets may exhibit fractionalized excitations similar to those which appear in the fractional quantum Hall effect. The interest in this phenomenon is generated by the increasing number of experimental results showing new physical behaviors in strongly correlated systems. For instance, the normal state of the high temperature superconductors does not exhibit electronlike quasiparticles in its spectrum. Recently, different scenarios were proposed for the realization of points with deconfined fractional excitations. Senthil *et al.* [3] proposed that a *deconfined quantum critical point* may describe the quantum phase transition (QPT) between a Néel ordered state and a VBC. In a second scenario based on models for quantum dimers, the deconfined point separates two VBC's and the spectrum of fractional excitations consists of spinless particles (''photons'') with a quadratic dispersion [4]. Very recently, Tsvelik [5] argued that none of the previous scenarios are realized for a family of frustrated spin Hamiltonians called confederate flag models [6]. As we will see below, his alternative scenario has many analogies with the case studied in the present Letter.

In addition, during the last decade attention has focused on the study of inhomogeneous structures that are proposed to emerge from competing interactions. These textures are generated by the proliferation and eventual ordering of one-dimensional (1D) topological defects. A prominent example is provided by the stripe phase proposed to exist in the high temperature superconductors. In this case, each stripe is an antiphase boundary for the AF order parameter. In general, it is difficult to prove the existence of these phases due to the complexity of the underlying frustrated model.

In this Letter, we will consider the $J_1 - J_2$ Heisenberg Hamiltonian on a square lattice with an additional term that makes the model quasiexactly solvable for the fully frustrated point $J_2/J_1 = 0.5$. At this point, some of the exact ground states are VBC's with deconfined fractional $S = 1/2$ excitations (spinons). In addition, spin-charge separation occurs if the system is doped with a low concentration of holes. We also show that this particular point has an emergent Z_2 gauge symmetry [7] and can be associated with a *first-order* QPT between two different VBC's. The physical manifestation of the emergent gauge symmetry is a divergent susceptibility for the creation of 1D topological defects that can be identified with twin boundaries of an underlying orientational ordering. The common origin of these exotic behaviors is a dynamical decoupling of the 2D magnet into 1D structures.

We will start by considering the following $S = 1/2$ Hamiltonian on a square lattice:

$$H = J_1 \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S_i} \cdot \mathbf{S_j} + J_2 \sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle} \mathbf{S_i} \cdot \mathbf{S_j} + K \sum_{\alpha} (P^{\alpha}_{ij} P^{\alpha}_{kl} + P^{\alpha}_{jk} P^{\alpha}_{il} + P^{\alpha}_{ik} P^{\alpha}_{jl}), \quad (1)$$

where $\langle \mathbf{i}, \mathbf{j}\rangle$ and $\langle\langle \mathbf{i}, \mathbf{j}\rangle\rangle$ denote nearest neighbors and second nearest neighbors, respectively. The index α denotes the sites of the dual lattice (plaquettes) and $ijkl$ are the

four spins of the corresponding plaquette in cyclic order. Note that the plaquette interaction of H is similar to the one introduced by a four cyclic exchange (the only difference is in the sign of the last term) [8]. In particular, we will consider here the fully frustrated point $J_2 = J_1/2$ and $K = J_1/8$. At this point, H can be rewritten as

$$H_p = \frac{3J_1}{2} \sum_{\alpha} \mathcal{P}^{\alpha}. \tag{2}$$

The operator $\mathcal{P}^{\alpha}$ projects the spin state of the plaquette α onto the subspace with total spin $S_T^{\alpha} = 2$.

Exact ground states of H_p.—It is clear that any state having at least one singlet dimer per plaquette is a ground state of H_p. This is because H_p is positive semidefinite and the condition of at least one singlet in the plaquette α implies that $S_T^{\alpha} \leq 1$ (no $S_T^{\alpha} = 2$ component). The same procedure gives rise to the Majumdar-Ghosh [9] and the Affleck-Kennedy-Lieb-Tasaki [10] exact ground states for $S = 1/2$ and $S = 1$ chains, and to more general ideas for constructing solvable 2D models [11,12].

We found two families of states that fulfill the condition of having at least one singlet dimer per plaquette. The first family is generated by the state which is illustrated in Fig. 1(a). These states are simply products of local singlet dimers which are represented by ellipsoids. In other words, the singlet dimers are completely localized and there is emergent U(1) gauge symmetry associated with this localization [7]. Any array of dimers along a given diagonal direction, $(1, 1)$ or $(1, \bar{1})$, can be rotated by $\pi/2$ as indicated by the arrows of Fig. 1(a). It is important to note that successive rotations have to be done along the same diagonal direction. The degeneracy of this family is 2^{N_d+1}, where $N_d \propto \sqrt{N_s}$ is the number of diagonal chains and N_s is the total number of sites. This degeneracy can be associated with a Z_2 gauge *emergent symmetry* that changes the dimerized order parameter of each individual diagonal zigzag chain. By Z_2 gauge symmetry we mean a local symmetry transformation that acts on each individual zigzag chain mapping one of the two possible dimerized states into the other one. Then, this family of ground states is formed by configurations with parallel diagonal arrays of vertical or horizontal dimers.

There is an alternative way of viewing the local Z_2 emergent symmetry. We can imagine that our system has an underlying orientational ordering given by the staggered dimer phase illustrated in Fig. 1(a). The two possible orientations are horizontal and vertical. The energy cost of a twin boundary or interphase between the two different orientations is zero. Consequently, the system has a divergent susceptibility for the creation of 1D topological defects, meaning that a weak coupling with another field can easily stabilize a particular array of twin boundaries. The ordering of 1D topological defects has been proposed as a possible outcome of competing interactions in the high-T_c superconductors [13].

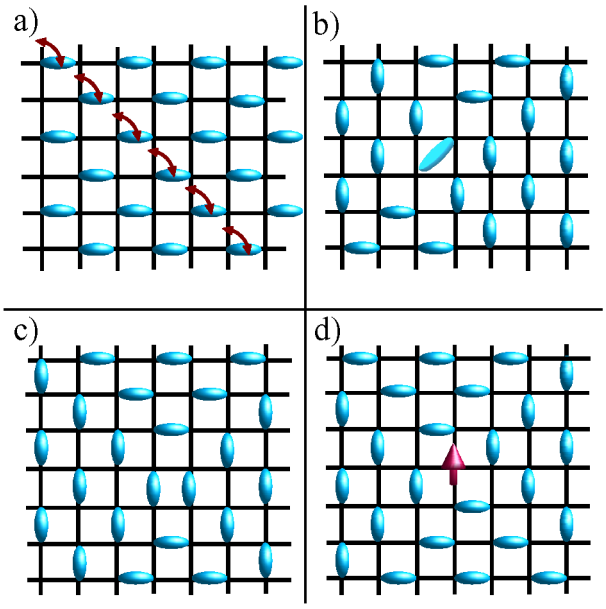

FIG. 1 (color online). Different ground states of H_p. The ellipsoids represent singlet dimers.

The second family [Figs. 1(b)–1(d)] appears when we force the states to have interfaces between vertical and horizontal configurations along the two diagonal directions $(1, 1)$ and $(1, \bar{1})$. Under this condition, the state is forced to create a defect at the intersection between the two diagonal interfaces. In particular, it is possible to have an $S = 1/2$ defect or localized *spinon* as is illustrated in Fig. 1(d). It is easy to prove that there is no ground state with more than one localized spinon. Since the position of the defect is arbitrary, the degeneracy of each of these configurations is proportional to N_s.

Deconfined fractional excitations.—What are the low energy excitations of the ground states of Fig. 1? Let us first consider the family of solutions illustrated in Fig. 1(a). As we can see in Fig. 2(a), if we excite one singlet dimer into a triplet state, the two parallel $S = 1/2$ spins can propagate along the diagonals without an energy cost proportional to the separation between them. Consequently, the two spinon excitations are *deconfined*. Note that when the spinons propagate along one diagonal zigzag chain they do not "see" the other chains because the two possible dimerized configurations (horizontal and vertical) have exactly the same energy. In other words, the effective dimensionality of the low energy spectrum is dynamically reduced from $D = 2$ to $D = 1$. The emergent Z_2 gauge symmetry that we mentioned above is the mathematical manifestation of this dynamical decoupling. The Z_2 dimerized order parameter of each diagonal zigzag chain is decoupled from the corresponding order parameter of the other chains. The most notorious physical consequence is the emergence of fractional excitations which are characteristic of 1D systems.

Note that the previous analysis is valid only when the spinons are moving along the two diagonal directions. If,

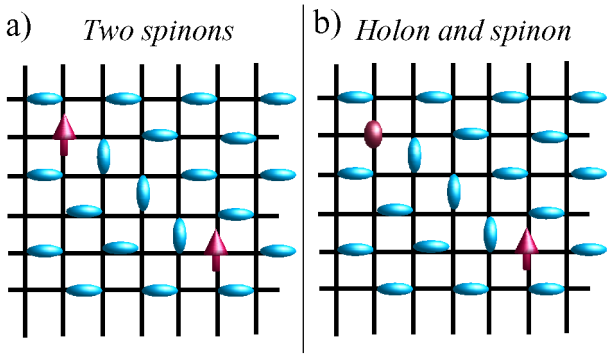

FIG. 2 (color online). Deconfined fractional excitations. (a) Two deconfined spinons. (b) Spin-charge separation when a low concentration of holes is introduced in the system.

for instance, they propagate horizontally, they will "feel" the confining interaction characteristic of 2D systems because the horizontal chains are not dynamically decoupled. Consequently, although our system is 2D, its low energy spinon excitations are free to move only along 1D paths. The same type of deconfined spinon excitations are obtained for the second family of ground states.

A similar situation occurs when one hole is introduced [Fig. 2(b)]. The charge and the spin of the hole get deconfined because there is no energy cost for the string generated in between the two excitations. Hence, we can expect a non-Fermi liquid behavior when a magnetic system described by H_p is doped away from half filling. These "exotic" behaviors are just a consequence of a dynamical decoupling which is signaled by an emergent Z_2 gauge symmetry and that occurs only at the point under consideration. To understand what can be the physical role of this point, we need to move away from it.

First-order quantum phase transition.—The special point described by H_p can be easily converted into a *first-order* QPT point. Note that the two configurations of Fig. 3 are the periodic ground states with the shortest periods. Therefore, they are the leading candidates to remain as ground states when we depart from the H_p point. For instance, we can add a term to the Hamiltonian which favors the *staggered* dimer ordering shown in Fig. 3(a) when the coupling constant g is negative or the *zigzag* dimer configuration of Fig. 3(b) when g is positive. There are different realizations of such a term and we will not focus in any particular one. The two different dimer phases shown in Fig. 3 break simultaneously the translation and the rotation symmetry of the square lattice. The first dimer configuration [Fig. 3(a)] is fourfold degenerate, while the second one [Fig. 3(b)] has an eightfold degeneracy. The order parameters are

$$\mathcal{D}^{\mathrm{st}}_{\eta} = \frac{1}{N_s}\sum_{\mathbf{j}} (\mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}+\hat{\eta}}) e^{i\mathbf{Q}\cdot\mathbf{r}_{\mathbf{j}}}, \tag{3}$$

for the staggered dimer ordering of Fig. 3(a) and

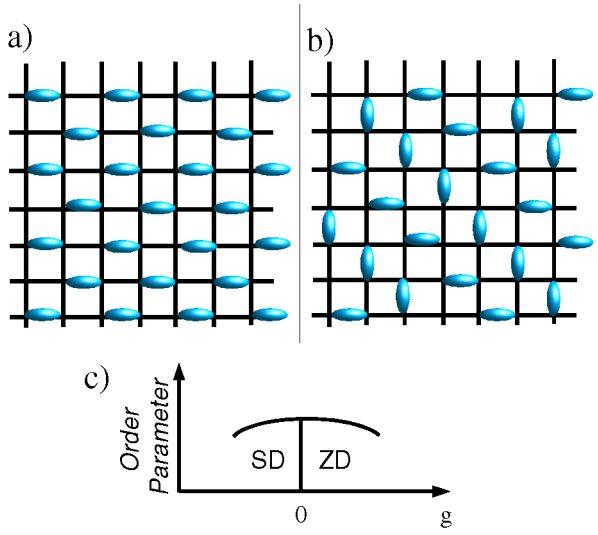

FIG. 3 (color online). (a) Staggered dimer phase (SD). (b) Zigzag dimer phase (ZD). (c) The two order parameters change discontinously at $g = 0$ indicating a first-order quantum phase transition between the phases illustrated in (a) and (b).

$$\mathcal{D}^{zz}_{x} = \frac{1}{N_s}\sum_{\mathbf{j}} (\mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}+\hat{x}} + \mathbf{S}_{\mathbf{j}+2\hat{\mathbf{x}}} \cdot \mathbf{S}_{\mathbf{j}+2\hat{x}+\hat{y}}) e^{(i/2)\mathbf{Q}\cdot\mathbf{r}_{\mathbf{j}}},$$
$$\mathcal{D}^{zz}_{y} = \frac{1}{N_s}\sum_{\mathbf{j}} (\mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}+\hat{y}} + \mathbf{S}_{\mathbf{j}+2\hat{\mathbf{y}}} \cdot \mathbf{S}_{\mathbf{j}+2\hat{x}+\hat{y}}) e^{(i/2)\bar{\mathbf{Q}}\cdot\mathbf{r}_{\mathbf{j}}}, \tag{4}$$

for the zigzag ordering of Fig. 3(b), where $\mathbf{Q} = (\pi, \pi)$, $\bar{\mathbf{Q}} = (\pi, -\pi)$, and $\eta = \{\hat{x}, \hat{y}\}$. Note that $(\mathcal{D}^{\mathrm{st}}_{x}, \mathcal{D}^{\mathrm{st}}_{y}) = (\pm 1, 0)$ or $(0, \pm 1)$ for the four equivalent ground states of the staggered dimer phase. For the zigzag phase, the nonzero component of $(\mathcal{D}^{zz}_{x}, \mathcal{D}^{zz}_{y})$ takes the four possible values $\{1, i, -1, -i\}$ that are necessary to identify the eight equivalent configurations. The remaining symmetry group of the zigzag phase, $\mathcal{G}^{zz}$, is a subgroup of $\mathcal{G}^{\mathrm{st}}$, the symmetry group of the staggered dimer phase. The level crossing that occurs at $g = 0$ between the staggered and the zigzag dimer states gives rise to a first-order QPT; i.e., there is a discontinuous change of the order parameters $\mathcal{D}^{\mathrm{st}}$ and $\mathcal{D}^{zz}$ [see Fig. 3(c)]. This level crossing is accompanied by the softening of the twin-boundary defects of the staggered dimer phase. Hence, we can think of the zigzag dimer phase as a "condensation" of these twin boundaries.

What is the general feature that gives rise to exotic behaviors? To answer this question it is convenient to think of our system as an array of diagonal zigzag chains. For each of these chains we can introduce the usual Z_2 dimer order parameter $\mathcal{D}_l$, where l is the chain index. We can now build different order parameters for the 2D system by choosing different periodic configurations of D_l with a well defined interchain wave vector k. For instance, in the case under consideration the dimer phase of Fig. 3(a) corresponds to the uniform ($k = 0$) configuration $\mathcal{D}_l = D$; i.e., the one-dimensional Z_2 order pa-

rameter points in the same direction for all the different chains. In contrast, the zigzag dimer ordering of Fig. 3(b) corresponds to $\mathcal{D}_l = (-1)^l D$; i.e., there is a staggered ($k = \pi$) interchain ordering. Since the different states built in this way have different wave vectors k, the QPT between two of them is of first order. At the transition point, both states have the same energy, meaning that there are adjacent chains for which the two relative orientations of D_l are degenerate. In other words, the effective coupling between these two chains has been reduced to zero and a Z_2 gauge symmetry emerges at the transition point. In general, we can say that these are QPT's between two broken symmetry states whose order parameters have something in common: given a particular decomposition of our 2D system into 1D chains described by some macroscopic variable, both order parameters characterize different interchain orderings.

For real systems, we do not expect the dynamical decoupling into 1D systems to be perfect. In general, there is always some residual interaction that makes this coupling weak but nonzero. A similar situation occurs in the materials that provide an experimental realization of one-dimensional systems. The structure of these materials contains weakly coupled chains and the coupling becomes relevant when temperature is lower than some characteristic value T_0 . However, the system still behaves as an array of decoupled chains for $T > T_0$. We expect the same behavior for 2D systems that get dynamically deconfined into 1D strucutures.

These ideas can be extended to other lattices. For instance, for a honeycomb lattice we can consider a Hamiltonian that is the sum of operators $\mathcal{Q}^\alpha$ that project the spin state of the plaquette α onto the subspace with total spin $S_T^\alpha = 2, 3$. As in the previous case, the system gets dynamically deconfined into chains that have two possible dimerized states. Consequently, there is an emergent Z_2 gauge symmetry that gives rise to the exotic behaviors which are described above.

Conclusions.—In summary, we obtained different exact ground states for a simple extension of the $J_1 - J_2$ Heisenberg model at the fully frustrated point $J_2/J_1 = 0.5$, $K = J_1/8$. The ground states and their low energy excitations exhibit exotic behaviors, such as the softening of 1D toplogical defects and the emergence of deconfined fractional excitations. When some of the spins are replaced by holes, the phenomenon of spin-charge separation occurs in the limit of low concentration of holes. In addition, the point under consideration can be identified with a first-order QPT.

Our model is an isotropic version of the anisotropic Confederate Flag model studied by Tsvelik [5]. By analyzing the four chain model, he finds that there are two VBC's separated by an approximately $(1 + 1)$ Lorentz invariant quantum critical point. However, the exponent that he obtains for the average dimerization is quite small, indicating that in the limit of infinite number of chains the transition could become first order as in the isotropic model discussed in this Letter. Our results then show that this phenomenon is not restricted to quantum critical points. In our case, the common origin of these deviations is a dynamical decoupling of the 2D magnet into 1D systems. This decoupling was proposed for 2D strongly correlated models in the context of the high temperature superconductors [14]. As is well known, this effective reduction of the dimensionality gives rise to completely different properties: the usual Fermi liquid is replaced by a Luttinger liquid and the magnetic spectrum is dominated by $S = 1/2$ spinon excitations.

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