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New class of frustrated quantum spin systems with an exactly known ground state

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We present a new class of quantum systems whose ground state can be found exactly. This construction involves an assembly of finite frustrated clusters connected by fixed spins. By contrast to solvable dimerized models, our systems exhibit long-range magnetic order, providing a striking example of ordering by quantum fluctuations in the presence of frustration.

Very few quantum spin systems can be solved exactly. Besides the class of one-dimensional integrable models,[1] it has been possible to find the exact ground state of some dimerized systems,[2] in one dimension or more.[3,4] Such models are defined on a hypercubic lattice, with some additional next-nearest-neighbor interactions. The lattice obeys the constraint that each nearest- and next-nearest-neighbor interaction belongs to at least one triangle. In such systems and for some range of the coupling strengths, the ground-state wave function is dimerized along the next-nearest-neighbor interactions. This result comes from the fact that any triangle with a strong enough antiferromagnetic bond and two equal remaining bonds has a dimerized ground state along the strongest bond. The third spin, in the spin-$\frac{1}{2}$ case, for instance, is free to be up or down, and is used to connect adjacent triangles.

In this Rapid Communication, we shall address the two following questions: Is it possible to use frustrated loops of any length instead of triangles only? What is the nature of the exact ground states which may then be generated? More precisely, we would like to know whether or not it is possible to have a free spin in the ground state of frustrated loop, besides the well-known triangle.

In the course of this investigation, the following definitions will be useful. Let us consider a finite cluster of n spins (for simplicity, we shall restrict ourselves to the spin-$\frac{1}{2}$ case). These spins are supposed to interact with the Hamiltonian of the following kind: $H=\sum_{ij}J_{ij}S_iS_j$. A given site i on the cluster is said to have a free spin if the ground state is degenerate and the corresponding wave function can be written as

$$|\psi\rangle = |S_i=\uparrow\rangle \otimes |\psi_\uparrow\rangle \text{ or } |\psi\rangle = |S_i=\downarrow\rangle \otimes |\psi_\downarrow\rangle ,$$

with $|\psi_\uparrow\rangle = |\psi_\downarrow\rangle$. Here $|\psi_\uparrow\rangle$ and $|\psi_\downarrow\rangle$ refer to the $n-1$ spins other than the spin at site i. We note that this definition agrees with the result for frustrated triangles. There, the site opposite to the strongest bond has a free spin.

As we shall show below, it is also quite useful to consider the situation where the ground-state wave function can be factorized as above, but with $|\psi_\uparrow\rangle \neq |\psi_\downarrow\rangle$. In this case, we shall say that the site i has a fixed spin (it is either up or down, but remains correlated with its neighbors). This is a weaker assumption on the possible ground state and arises naturally while trying to generalize the concept of free spin.

At the beginning of this discussion, we show that it is impossible to have an isolated fixed or free spin in an open chain. We exhibit then simple systems with one and two loops and one and two isolated fixed spins, respectively, which cannot be decomposed into a combination of elementary triangles. They are used then to construct infinite frustrated models with an exactly known ground state. A generalization to finite clusters with any number of fixed spins is also discussed. Our models illustrate a new type of behavior arising from the interplay between frustration and quantum fluctuations, which has no classical counterpart at zero temperature.

Let us first investigate the possibility of constructing a finite one-dimensional system, whose ground state contains free or fixed spins. A positive answer to this question would give us the opportunity to find the exact ground-state wave function for a class of one-dimensional systems without loops. Unfortunately, in the presence of any number of antiferromagnetic interactions it is impossible to construct such systems as we shall prove.

Let us consider an open chain as shown in Fig. 1. The Hamiltonian is chosen to be $H=\sum_i^{n-1}J_iS_iS_{i+1}$. Suppose there is a free and/or fixed spin on a given site. The ground-state wave function may be written as

$$|\psi\rangle = |\psi_L\rangle \otimes |\uparrow\rangle \otimes |\psi_R\rangle = |\psi_L^{\sigma_L}\rangle \otimes |\sigma_L \uparrow \sigma_R\rangle \otimes |\psi_R^{\sigma_R}\rangle , \quad (1)$$

where $|\psi_L\rangle = \sum_{\sigma_L} |\psi_L^{\sigma_L}\rangle \otimes |\sigma_L\rangle$ and the same for the right side. The condition that $|\psi\rangle$ is an eigenstate leads to

$$J_L |\psi_L^{\downarrow}\rangle \otimes |\psi_R^{\uparrow}\rangle + J_R |\psi_L^{\uparrow}\rangle \otimes |\psi_R^{\downarrow}\rangle = 0 , \quad (2)$$

$$|\psi_L^{\downarrow}\rangle \otimes |\psi_R^{\downarrow}\rangle = 0 . \quad (3)$$

So, $|\psi_L^{\downarrow}\rangle = 0$ or $|\psi_R^{\downarrow}\rangle = 0$. Let us assume that $|\psi_L^{\downarrow}\rangle = 0$ and $|\psi_R^{\downarrow}\rangle \neq 0$. Then from the first equation, we get $|\psi_L^{\uparrow}\rangle = 0$, so $|\psi_L\rangle = 0$ and $|\psi\rangle = 0$. From this we deduce that both $|\psi_L^{\downarrow}\rangle$ and $|\psi_R^{\downarrow}\rangle$ vanish. Hence, $|\psi\rangle$ may be

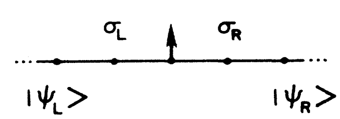

FIG. 1. σ_R and σ_L indicate the adjacent right and left spins to the fixed up spin. $|\psi_R\rangle$ and $|\psi_L\rangle$ represent the wave functions of all the right and left spins.

written as

$$|\psi\rangle = |\psi_L^{\uparrow}\rangle \otimes |\uparrow\uparrow\uparrow\rangle \otimes |\psi_R^{\downarrow}\rangle . \tag{4}$$

This shows by iteration that $|\psi\rangle$ is a ferromagnetic state. As a result, the presence of loops is necessary in order to have free and/or fixed spins in a system with some antiferromagnetic couplings. It is worthwhile to note that the same property holds also in the presence of anisotropic couplings or for any spin S. The proof as shown above can be adapted without any difficulty to these more general situations. However, we should note that this property breaks down in the presence of an external magnetic field and an anisotropic coupling. Indeed it has been shown that the XYZ spin-$\frac{1}{2}$ chain may have a classical alternating ground state, for some special values of the field.[5,6] In our discussion, we shall restrict ourselves to systems in zero field. Our motivation is to concentrate on the effect of frustrated loops in stabilizing a simple ground state.

The next simple cluster, besides a triangle, is a loop which consists of four spins $\frac{1}{2}$. One can verify that there is no way to choose interaction strengths which give a ground state with a free and/or fixed spin in a presence of antiferromagnetic interactions.

The next simplest cluster to be examined is a loop consisting of five spins $\frac{1}{2}$ as presented in Fig. 2. The Hamiltonian for this cluster is

$$H = \gamma S_1(S_2+S_5) + \alpha(S_2S_3+S_4S_5) + \beta S_3S_4 .$$

One can verify that one of the eigenstates of the system is given by

$$|\psi\rangle = |\uparrow\rangle \otimes [A_1(|\uparrow\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\uparrow\rangle) + A_2(|\uparrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle)] \tag{5}$$

where the coefficient A_1 is given by

$$A_1^{-2} = 4\left\{1 + \frac{(\gamma-2\beta)^2}{4\alpha^2}\left[1+\left(1+\frac{4\alpha^2}{(\gamma-2\beta)^2}\right)^{1/2}\right]\right\}, \tag{6}$$

and $A_2^2 = 1 - A_1^2$. Numerical solutions of the whole spectrum of this system show that there is a *finite* fraction of the volume in the (α,β,γ) space, in which the eigenstate equation (5) is the ground state of the system. A typical range of β and γ for a fixed positive α is presented in Fig. 3. A similar picture can also be found for the case of negative α.

The solution of this system indicates a few important results. (i) It is possible to have a fixed spin in loops with a length greater than three. (ii) Unlike the triangular case, the ground-state wave function is a linear combination of *singlets and triplets* between the pairs of spins (2,5) and (3,4) [see Eq. (5)]. (iii) The total spin of the wave function in Eq. (5) is $\frac{3}{2}$. Therefore, the total spin of the ground-state wave function in a presence of a fixed spin could be greater than the minimal spin value. (iv) In all the volume with the ground state in Eq. (5), the loop is frustrated. The two (from four possibilities) possible frustrated loops are $\alpha<0$, $\beta>0$, and $\gamma<0$ or $\alpha>0$, $\beta>0$, and $\gamma<0$. (v) Decreasing the value of γ for a fixed values of α and β, the ground-state wave function changes its total spin.

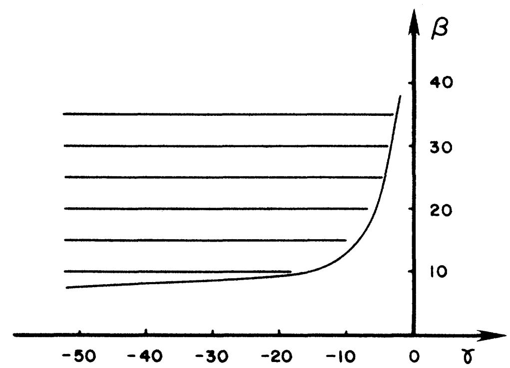

FIG. 3. The dashed area indicates the range in the subspace (α, β, γ) with $\alpha=8$, in which the ground-state wave function is given by Eq. (5).

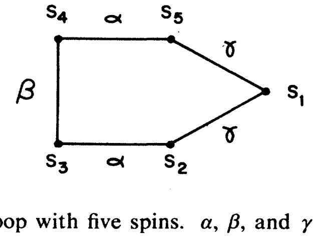

FIG. 2. A loop with five spins. α, β, and γ stand for the interaction strengths.

As it has been done for frustrated triangles, which have one free spin, we may try to use the previous five-spin ring with one fixed spin, in order to construct an infinite system which ground state can be found exactly. However, there is a major difference between free spins and fixed spins. A free spin can be used to connect any two clusters, but a fixed spin has to be connected to another fixed spin or a free spin.

Infinite systems connected via free spins have short-range spin-spin correlation functions. This is the case for instance in dimerized chains.[2] One may also construct infinite systems involving fixed spins and free spins as well, as shown in Fig. 4(a). In this case, the ground state is infinitely degenerate, since the fixed spins belonging to different pentagons can be assigned any given pattern. This finite entropy prevents the system from developing true long-range order.

An important difference arises if it is possible to find a finite cluster with at least two fixed spins. Then, by connecting identical clusters using those fixed spins, one gets a model with a known ground state, and without any free spin. We shall now discuss how the previously studied system can be used to generate more complex geometries with several fixed spins.

The first possibility is to combine two pentagons in a two-loop cluster of eight spins as shown in Fig. 4(b). When β is positive and very large, the ground state has a singlet bond between the spins S_A and S_B. When some weak ferromagnetic couplings ($\alpha<0$, $\gamma<0$) are turned on, this singlet bond is expected to remain strong. The

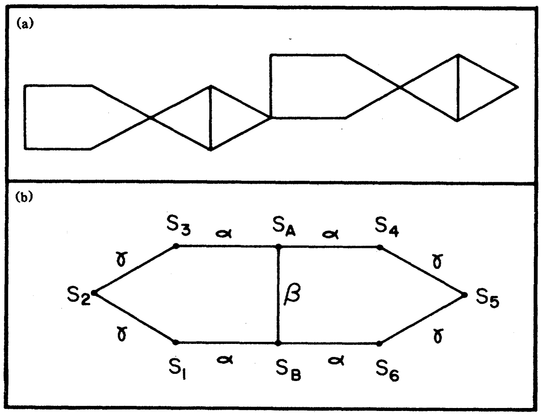

FIG. 4. (a) A part of an infinite one-dimensional system, with a solvable ground state. The right spin in each pentagon's ground state is a fixed spin, see Eq. (5). The interactions in each pair of adjacent triangles are chosen such that the ground state of this subsystem is dimerized along the common edge with remaining two free spins (Ref. 3). The scale of the interactions is chosen to be such that the ground state of each pentagon is the same and equal to the ground state of each pair of triangles. (b) A combination of two pentagons in a two-loop cluster of eight spins.

ground state has an odd parity in the reflection around the (2,5) axis, and has total spin 3. It can be represented by a state with one down spin and seven up spins, in which the down spin avoids sites 2 and 5 (because of the parity). Thus, we expect to get two parallel fixed spins at sites 2 and 5 in this large-β limit.

In order to show that this indeed happens, it is interesting to look at the perturbation theory when α/β and γ/β are both small.

If $\gamma/\beta=-\epsilon$ and $\alpha/\beta=-\lambda\epsilon$, the Hamiltonian can be written as

$$H/\beta=H_0+\epsilon V,\quad V=V_0-\lambda U,\quad H_0=S_A S_B\,, \tag{7}$$

where

$$V_0=-(S_1S_2+S_2S_3+S_4S_5+S_5S_6)$$

and

$$U=S_A(S_3+S_4)+S_B(S_1+S_6)\,.$$

We have to select the subspace L_0 for which S_A and S_B are in a singlet state (to minimize H_0), and the sites 1,2,3 and 4,5,6, respectively are in the ferromagnetic state $S=\frac{3}{2}$ (to minimize V_0). This subspace is spanned by four possible values of the total spin, from 0 to 3. The degeneracy between those four subspaces is lifted only at order ϵ^3. After lengthy calculations we obtain

$$E/\beta=-3/4-\epsilon-\lambda^2\epsilon^2/2+(\lambda^2/4+a\lambda^3+b\lambda^4)\epsilon^3+O(\epsilon^4)\,. \tag{8}$$

The $b\lambda^4\epsilon^3$ term comes from the fact that U^2 acting on a state in L_0 induces transitions to some states in which the total spin for the 1,2,3 and 4,5,6 clusters is no longer $\frac{3}{2}$ but $\frac{1}{2}$. This modifies the first-order correction to the eigenstate by a factor $\lambda^2\epsilon$. The values of a and b for $S=3,2,1,0$ are $-\frac{1}{4}$, $\frac{1}{12}$, $\frac{11}{36}$, $\frac{5}{12}$ and $0,0,-\frac{5}{18},-\frac{1}{2}$, respectively. So, when ϵ is small, and λ is not too large, the ground state has a total spin 3, and an odd parity with respect to the (2,5) axis. This proves the existence of the two fixed spin configuration in some region of the parameter space.

It is now possible to combine these eight spin clusters into a quasi-one-dimensional system by joining the extremities (sites 2 and 5) of two nearest-neighbor clusters. When the parameters α, β, and γ are such that the ground state of a given cluster has two fixed spins, the ground state of the "polymerized" system is easily built by taking tensor products of the ground-state wave function inside each cluster. In this situation all the sites connecting adjacent elementary cells have parallel fixed spins. This system has then long-range order, since the spin-spin correlation functions do not decay at large separations. The low-lying excitations in the presence of a periodic succession of fixed spins are likely to be similar to the long-wavelength spin waves in a ferromagnet, since the total spin of a given cluster is nonzero, allowing for an infinitesimal twist along the chain.

This is a simple example of "ordering by quantum fluctuations" in a frustrated system. Classically, there is a finite entropy per spin at zero temperature when β is large. Quantum fluctuations lift this infinite degeneracy and select a ground state which exhibits long-range magnetic order. We have here a simple example for which a quantum system and its classical version behave quite differently. A somewhat similar mechanism has been discussed by Fazekas and Anderson.[7,8] They have shown that for a strongly anisotropic spin-$\frac{1}{2}$ antiferromagnetic Hamiltonian on the triangular lattice, quantum fluctuations drive the system into a resonating-valence-bond ground state which exhibits some phase rigidity. However, in this case, such a rigidity did not lead to any long-range order.

One can easily generalize the case of a cluster with two parallel fixed spins to a case of two antiparallel fixed spins. For instance, assume that J_{45} and J_{56} [in Fig. 4(b)] are changed to anisotropic interactions such that $J_{45}^x=-J_{45}^y=-J_{45}^z=J_{56}^x=-J_{56}^y=-J_{56}^z=\gamma$. It is obvious that this system is identical to the previous isotropic system after the action of π rotation along the x axis on the spin S_5. Therefore, the ground state of the system consists of two antiparallel fixed spins. It is now obvious that one can combine these eight spin clusters into a quasi-one-dimensional system where the extreme spins are in any possible order.

Let us now briefly discuss how our mechanism may be generalized to higher dimensions. In order to construct a n-dimensional array, it requires finite clusters with $2n$ fixed spins. From the two previously discussed geometries, the maximal number of fixed spins on a finite cluster appears to be related to the number of independent loops on the graph associated to the J_{ij} matrix. (Here, we are still looking at possible ground states which are not simply ferromagnetic.) We would like to argue that those two numbers are actually equal. Indeed, let us consider multiconnected clusters, on which possible fixed spins are not located at vertices. We have then the three following properties: (1) Each fixed spin belongs to a closed path on the graph which does not contain any other fixed spin. (2) A set of points on a cluster which satisfies property (1) may be called an admissible set of spins. Then, for a graph with n-independent loops, the number of sites of any admissible set is less or equal to n. (3) For a graph with n-independent loops, there exists an admissible set containing n sites.

Properties (2) and (3) are purely geometrical and can be proved by induction on the number of independent loops. If property (1) is not satisfied, it is possible to find a fixed spin such that any path originating from it is obstructed by another fixed spin. So the system contains at least two uncorrelated parts separated by a fixed spin. Following the same reasoning as for the open chain, we find that the fixed spin propagates along each side of the initial one, and that the whole system becomes ferromagnetic.

Of course, the existence of an admissible set of spins is only a necessary condition for the existence of isolated fixed spins. An explicit algorithm to construct a n fixed-spin ground state for a given n-independent loop cluster has still to be found. However, the two examples above suggest that such a generalization is certainly possible.

To conclude, we have presented some finite systems which exhibit a remarkable ground state, characterized by the presence of one or several fixed spins. These systems are all frustrated. However, we should stress that the properties of these fixed spins are quite different from those of free spins which have been considered for instance in the dimerized models. Free spins appear only in frustrated triangles, but fixed spins can be found in large loops. Furthermore, the spin background is in a singlet state in the case of a free spin, whereas for the fixed spin, the total spin is not expected to vanish. This provides an explicit example of a system in which the total spin is finite, but smaller than in the fully polarized state.

We would like to note also that the fixed spins survive after a small modification of the Hamiltonian on a given cluster. So, our mechanism of ordering by quantum fluctuations is stable against some weak disorder in the couplings.

Is it possible to have isolated fixed spins for a large value of the spin S? How to describe the intermediate regime between the $S=\infty$ and $S=\frac{1}{2}$ limits? These questions certainly deserve further studies and may help to sharpen our understanding of the subtle interplay between quantum mechanics and frustration.

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