

results. Finally, with an increase in temperature, we observe an overall broadening and gradual decrease in the intensity of the spin-wave peaks. No qualitative change in the spectra was observed on cooling the sample through T_N at 23 K.

In summary, we have established a band of spin-wave excitations in 1D Ising-type antiferromagnetic system. These excitations seem to be related to the motion of domain-wall pairs in the chain. The motion of domain walls should also be manifested in the central component of the $S_{zz}(Q, \omega)$ response function. It was first predicted by Villain¹¹ that at low temperatures the spin dynamics of an antiferromagnetic linear chain can be governed by propagation of thermally excited domain walls. Such a problem is presently under investigation.

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Renormalization-Group Study of a Two-Dimensional Frustratedlike Quantum Spin System

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The ground-state properties of a generalized quantum $s = \frac{1}{2}$ XY model (including the ferromagnetic and antiferromagnetic cases) in a Z field on a triangular lattice are examined. The exact values of critical fields above which the gap opens are obtained. A real-space renormalization-group method is used to estimate the ground-state energy and to analyze the critical behavior. There is some evidence that certain features of frustration in classical spin systems still persist in quantum systems.

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We consider a generalized spin- $\frac{1}{2}$ planar quantum model with a transverse field:

$$H = -(J/2) \sum_{i,j,n,n'} [\cos\theta(S_i^x S_j^x + S_i^y S_j^y) + \sin\theta(S_i^x S_j^y - S_i^y S_j^x)] - \hbar \sum_i S_i^z, \quad (1)$$

where $\hbar > 0$, $J > 0$, $S^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, etc., and θ is a parameter. The nearest-neighbor interaction in (1) is a quantum extension of the classical interaction $-J \cos[\theta - (\varphi_j - \varphi_i)]$ which is minimum when the angle $\varphi_j - \varphi_i$ between neighboring spins is θ . (For $\theta \neq 0$ or π , it is necessary to introduce a conventional orientation $i-j$ of each bond.)

For $\hbar = 0$, Hamiltonian (1) includes, as special cases, the ferromagnetic (F) XY ($\theta = 0$) and the antiferromagnetic (AF) XY ($\theta = \pi$) models; it

also includes for $\theta = \pi/2$, the Dzialoshinsky-Moriya (DM) model which was introduced, along with the XY model, to describe the weak ferromagnetism (but, to date, only for classical spins). On bipartite lattices, our model is equivalent to the FXY model (it suffices to rotate each spin of one sublattice by θ). The study of (1) becomes very interesting on nonbipartite lattices, which give rise to "frustration" for classical AF Ising

interactions, a typical example being the triangular lattice.

The study of frustration in quantum systems started when Anderson¹ suggested analysis of the nature of the ground state (G.S.) of the AF $s = \frac{1}{2}$ Heisenberg model on a triangular lattice where Néel-type antiferromagnetic order should be replaced by a liquid-type order.¹ We have recently done a renormalization-group calculation of the AF Ising model on the triangular lattice, with a transverse field h .² We have found that the characteristic "frustrated" properties of the classical ($h = 0$) model³ persist up to a critical field $(h/j)_c \approx 1.41$, which is strongly reduced compared with the F value $(h/J)_c \approx 5$.⁴ It is therefore tempting to study another quantum model which does not display the Ising symmetry: the $s = \frac{1}{2}$ XY model, or a generalization thereof, Eq. (1), whose G.S. is completely unknown for all θ . Mattis⁵ has pointed out that on nonbipartite lattices, the G.S. of the AF XY model could be different from that of the FXY model. More recently, Marland and Betts⁶ investigated the G.S. of the AF XY model on a triangular lattice by extrapolating from exact finite-cell calculations. They observed an important increase of the G.S. energy compared to the F case, but they emphasized a difference with classical systems: The degeneracy of the G.S. is not greatly increased here.

The purpose of this Letter is to announce the results of an extended analysis of Eq. (1) on the triangular lattice for finite fields and for different degree of frustration, introduced here *gradually* by varying θ . We present the evidence that on going from F to AF situations, several effects reminiscent of frustration in classical systems appear: a general shrinkage of the low-energy spectrum reflected by (a) strong reduction (by factor of 2) of the critical ratio $(h/J)_c$ above which a gap opens, (b) an important increase of the G.S. energy (for $h = 0$, $-E_0/N \sim 1.5$ and 0.88 for F and AF, respectively). The central result here is that (c) the fully frustrated AF case [and equivalent situations $\theta = \pi/3 \pmod{2\pi/3}$, see below] has its scaling properties peculiar to its own nature, whereas *any* other situation, including intermediate cases like DM, etc., has the properties of the F case. In addition, (d) an increase of density of states near the bottom of the energy spectrum, reflected by a larger exponent z (where z tells how energy scales with length), and an increase of the decay rate of spin corre-

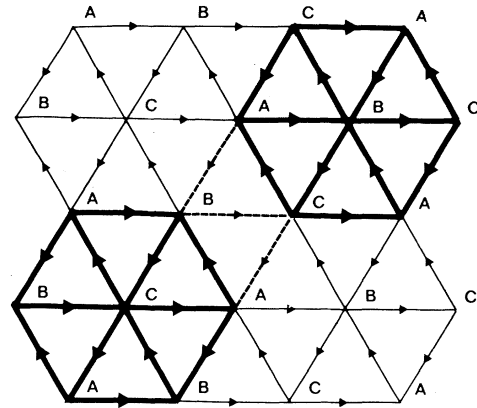


FIG. 1. The triangular lattice in 2D with the conventional orientation of the bonds and the three sublattices A , B , C used in text. Also shown are two adjacent blocks used for the renormalization-group calculations with their intrablock (thick lines) and interblock (dashed lines) couplings.

lations (larger exponent η) appear.

Before presenting the calculations let us specify that on the triangular lattice the bonds have been oriented as in Fig. 1 to define unambiguously the sign of the antisymmetric part of (1). Also all the properties of (1) will depend on θ with period $2\pi/3$: Rotate the spins on sublattices A , B , C of Fig. 1 by, respectively, 0 , $+2\pi/3$, $-2\pi/3$; then (1) maps on itself by changing θ into $\theta + 2\pi/3$. In particular $\theta = \pi/3$ is equivalent to the AF case, so that, by simply varying θ from 0 to $\pi/3$, we go continuously from the unfrustrated to the fully frustrated situation.

The critical field is obtained by equating the G.S. energies $E_N = -Nh$ and $E_{N-2} = e_{N-2} - (N-2)h$ of the two subspaces $\sum_i^N S_i^z = N$ and $\sum_i^N S_i^z = N-2$. Thus, we find $h_c = -e_{N-2}/2$, where e_{N-2} denotes the lowest energy, for $h = 0$, in the subspace $\sum_i^N S_i^z = N-2$. The calculation of e_{N-2} is standard (it is similar to finding the edge of a conduction band for an electron hopping on a triangular lattice). Considering a parallelogram of N_1 rows and N_2 columns, we can express any wave function ψ in the one-spin deviation subspace as a combination of the functions $\varphi_{i,j}$ which correspond to a spin flip located at row i and column j : $\psi = \sum a_{ij} \varphi_{i,j}$. After writing that ψ must be an eigenvector of H we find a set of coupled equations for the a_{ij} 's which can be solved after a Fourier transformation, by assuming periodic boundary conditions. We then get the whole energy spectrum in this subspace:

$$\epsilon_{N-2}(k_1, k_2) = -2J \{ \cos(k_1 - \theta) + \cos(k_2 - \theta) + \cos(k_1 + k_2 + \theta) \}, \quad (2)$$

where $k_i = 2\pi n_i/N_i$ ($i = 1, 2$), $n_i = \{-N_i, -N_i + 1, \dots, N_i - 1\}$. After minimizing, we find e_{N-2} and

$$(h/J)_c = 3 \cos(\theta - 2n\pi/3) \text{ for } (2n-1)\pi/3 < \theta < (2n+1)\pi/3. \quad (3)$$

The curve giving $(h/J)_c$ as a function of θ is plotted in Fig. 2 (full upper curve). In the F case [$\theta = 0 \pmod{2\pi/3}$] we recover the exact result.⁷ We observe that $h_c(\text{AF}) = 0.5h_c(\text{F})$.

The calculations of the G.S. energy ($h=0$) and of the critical behavior were performed with use of a recent renormalization-group method well suited for quantum systems.⁸ Since here [$H, \sum S_i^z$] = 0, we have followed closely the procedure used for the one-dimensional (1D) XY model⁹ and for the 2D XY model on several lattices.¹⁰ Here, the lattice is split into adjacent hexagonal blocks of $n_s = 7$ sites, coupled together by three original bonds, their centers forming a new triangular lattice dilated by $f = \sqrt{7}$. At each step of the iterative procedure we solve the Hamiltonian exactly for one isolated block and we retain the lowest two states of energies E_+ and E_- to define a new spin per block. For $h=0$, these states are degenerate and belong^{5, 9, 10} to the subspaces

$$\sum_{\text{block}} S_i^z = \pm 1.$$

But, when searching the critical field location, we must consider^{9, 10} the G.S. of the subspaces

$$\sum_{\text{block}} S_i^z = +5 \text{ and } +7.$$

Then, in both cases, by expressing the old spin operators in terms of the new block-spin operators we can get spin recursion relations necessary to rewrite the original interblock couplings. If we drop a constant term $\frac{1}{2}(E_+ + E_-)^{(n)}$, the Hamiltonian can be rewritten always in the same form and we can derive implicitly the recursion relations giving $h^{(n+1)}$, $J^{(n+1)}$, $\theta^{(n+1)}$ as functions of $h^{(n)}$, $J^{(n)}$, $\theta^{(n)}$, which can be iterated up to a "fixed-point" Hamiltonian. For any initial values of $h^{(0)}$, $J^{(0)}$, $\theta^{(0)}$ we observe that $\theta^{(n)} \rightarrow 0 \pmod{2\pi/3}$ except if $\theta^{(0)} = \pi/3 \pmod{2\pi/3}$, where $\theta^{(n)}$ remains constant. Thus, in the case $h=0$, where θ is the only relevant parameter, $\theta = 0 \pmod{2\pi/3}$ and $\theta = \pi/3 \pmod{2\pi/3}$ are, respectively, stable and unstable fixed points. On the other hand, when dealing with the renormalization-group transformation constructed from the subspaces

$$\sum_{\text{block}} S_i^z = +5 \text{ and } +7,$$

we find a critical curve $(h/J)_c$ reported in Fig. 2 (dashed curve). The comparison with the exact curve (full curve) gives an idea of the approxima-

tions. Also on the critical line, $\theta = 0 \pmod{2\pi/3}$ is stable while $\theta = \pi/3 \pmod{2\pi/3}$ is unstable. This leads to a crossover phenomenon. The crossover exponent Φ for $h = h_c$, $\theta = \pi/3$, which compares the instability in θ with the instability in h/J , is found to be $\Phi = 1.38$. A more detailed analysis of both the region $0 < h < h_c$ and the crossover phenomenon for θ close to $\pi/3$ will be described elsewhere.¹¹

The critical exponent z telling how the energy scales is deduced from the renormalization of J at the fixed point: $z = -\ln\{J^{(n+1)}/J^{(n)}\}/\ln f$. The exponent η giving the power-law decay of the spin correlation function, $\langle S_i^x S_{i+R}^x \rangle_{R \rightarrow \infty} \sim R^{-\eta}$, is estimated as in Refs. 2, 9, and 10, from the renormalization-group transformation of a spin average over the block. We give the results for z and η in Table I for the four interesting situations $h = 0$, $\theta = 0$ and $\theta = \pi$; $h = h_c$, $\theta = 0$ and $\theta = \pi$. As in the ferromagnetic case¹⁰ the exponents at $(h/J)_c$ are larger than those for $h=0$. But the most important point to be noticed is that the AF exponents are larger than corresponding F ones, reflecting the peculiar scaling properties of this fully frustrated situation.

The G.S. energy per site was evaluated by cumulating the constant terms $(E_+ + E_-)^{(n)}/2$ divided

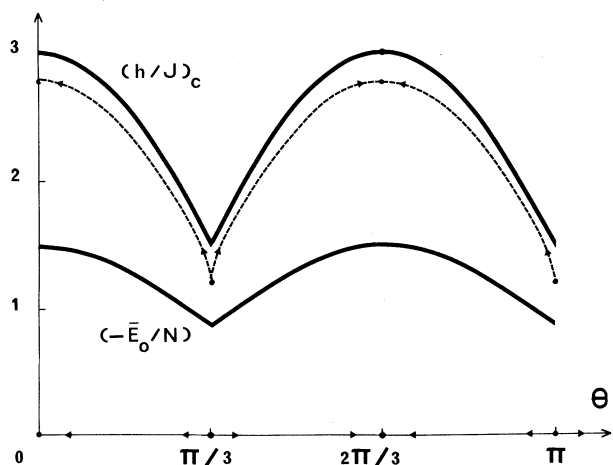


FIG. 2. Exact results for the critical field (full upper curve), and renormalization-group results for the critical field (dashed upper curve) and for the G.S. energy per site.

TABLE I. Exact and renormalization group (R. G.) results for the location of the critical field and R. G. results for the G. S. energy per site and for the critical exponents, in the two F ($\theta = 0$) and AF ($\theta = \pi$) cases.

θ	$(h/J)_c$		$(-\bar{E}/N)_{h=0}$	$h = 0$		$h = h_c$	
	Exact	R. G.	R. G.	z	η	z_c	η_c
0 (F)	3	2.78	1.50	0.045	1.21	1.09	2.04
π (AF)	1.5	1.20	0.88	2.03	3.04	1.84	2.16

by the number of sites at each step which is 7^{n+1} :

$$-\frac{E}{N} = \frac{1}{2} \sum_{n=0}^{\infty} \frac{E_+^{(n)} + E_-^{(n)}}{7^{n+1}}. \quad (4)$$

In the case of a small compact block, such as that used here, which does not retain the ratio b_s between the number of sites and bonds of the infinite lattice, (4) gives only a lower-bound estimate of the G.S. energy. An alternative (upper bound) estimate is obtained by dividing instead by the number of bonds at each step, $3 \times 7^{n+1} - 3^{n+2}$, and then multiplying the result by $b_s = 3$:

$$-\frac{E'}{N} = \frac{1}{2} \sum_{n=0}^{\infty} \frac{E_+^{(n)} + E_-^{(n)}}{7^{n+1} - 3^{n+1}}. \quad (5)$$

The arithmetical average between these two estimates, $-\bar{E}/N = -1/2(E + E')/N$, gives generally good results in 2D when comparing with other estimates.¹⁰ Here, the curve giving $-\bar{E}/N$ as a function of θ is reported in Fig. 2 (full lower curve). We find $-\bar{E}/N \approx 1.5$ and 0.88 for $\theta = 0$ and $\theta = \pi$, respectively, in reasonable agreement with the previous estimates of Marland and Betts⁵ ($-E/N = 0.9$ in the AF case). But more characteristic is the shape of the whole curve $-N^{-1}\bar{E}(\theta)$, which follows that of $(h/J)_c$, showing the general effect of frustration, i.e., a general shrinkage of the energy spectrum near the bottom of the continuum revealed by a strong reduction of both the critical field and the absolute value of the G.S. energy.

It is instructive to compare our results with the properties of the classical (spin ∞) AF XY model on a triangular lattice. Here also the G.S. energy is raised and the nature of the G.S. is more complicated than in the F case¹² while the classical DM model maps onto the F situation.

The question of the existence of long-range order in the G.S. for this quantum model is still difficult to answer. Our renormalization-group calculations give here no long-range order (for any θ) while finite cell calculations for the F XY $s = \frac{1}{2}$ model on 2D lattices suggest long-range order.¹³

This renormalization-group study will be ex-

tended to other spin systems such as the Heisenberg spin- $\frac{1}{2}$ AF model on a triangular lattice. It can be also extended to quantum systems on other types of 2D or 3D fully frustrated lattices and on partially frustrated regular or disordered lattices.

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