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Zero-temperature renormalization-group method for quantum systems. V. Frustration in two dimensions

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The ground-state properties of a generalized quantum $s=(1/2)$ XY model with symmetric and antisymmetric [Dzialoshinsky-Moriya (DM) type] interactions with a Z field on different planar lattices are examined. The parametrization of the model allows the interpolation between ferro- (F) and antiferromagnetic (AF) couplings through all the intermediate cases. The presence of DM terms necessitates the introduction of orientation of bonds. The different orientation conventions for different lattices are discussed. For a given convention and lattice the exact values of critical fields above which the gap opens are obtained. The real-space renormalization-group method is used to estimate the ground-state energy and to analyze the critical behavior. By going from F to AF situations the quantum frustration is reflected by a general shrinkage of the low-energy spectrum characterized by a strong reduction of critical fields and important increase of the ground-state energy. The fully frustrated case has special critical properties, while any other situation, including the DM interaction has the properties of the F case. Possible extensions to other relevant frustratedlike cases are indicated.

I. INTRODUCTION

This paper is a continuation of a series of papers[1–8] in which a newly developed real-space renormalization-group method[9,10] for quantum systems was applied to study the ground-state properties of a number of uniform spin models. In a separate series the disordered quantum systems,[11,12] the Yang-Lee singularity,[13,14] fermion,[15,16] and coupled spin-fermion[17] systems are being studied. There is a growing interest for the phase transitions in quantum systems and several extensions and modifications of the above method are at present under study.[18]

In this paper we shall present the calculations using a quantum model system whose ground-state properties are similar to those of certain classical systems, which display a phenomenon currently referred to as frustration. The study of such a classical frustrated system started from a pioneering work of Wannier.[19] He had proven exactly the impossibility of antiferromagnetic ordering on a triangular lattice. By going from ferromagnetic (F) to antiferromagnetic (AF) couplings the doubly degenerate Ising ground state goes over into an infinitely degenerate ground state with a finite entropy and without any order. The ground-state energy per spin increases from $-3J$ to $-J(J>0)$, the ordering does not reappear at $T>0$ and the $T=0$ spin-correlation functions have a characteristic power-law behavior.[20]

The appearance of infinitely degenerated, "frustrated" ground states, with peculiar critical properties and completely supressed ordering is a characteristic feature of numerous models of uniform, disordered, and impure systems.[19–23] In general, a system with uniform coupling constants may possess a frustrated ground state if the interaction is not compatible with the geometry of the underlying lattice. In the above example the two-body AF interaction is not compatible with the triangular lattice which has three sublattices. In contrast, the three-body interactions on the triangular lattice show a well-behaved transition at finite temperature[24] and the degeneracy of the ground state is small and does not depend on the number of spins in the system. On the other hand, even a two-body interaction on a square lattice may produce some sort of frustration effect if the two sublattices will be made inequivalent (see below).

The study of frustration in quantum systems has been initiated by Anderson[21] who pointed out a peculiar nature of the ground state of $s=\frac{1}{2}$ AF Heisenberg model on a triangular lattice. The subsequent studies extended these ideas to several other related problems.[25] However, the complexity of quantum systems for $D>1$ and a lack of knowledge about their ground states hampered the systematic investigations. Because of expected degeneracies the perturbative approaches to quantum frustration cannot be very effective.

It is only very recently that some new studies of this problem were undertaken. Mattis[26] pointed out that the ground state (GS) of the $s=\frac{1}{2}$ AF XY model on nonbipartite lattices could be very different from that of the F model. This observation has been confirmed by the calculation by Betts and Marland[27] of the GS energy of the $s=\frac{1}{2}$ AF XY model on a triangular lattice. They have used the method of extrapolating from exact finite-cell calculations. An important increase of the GS energy as compared to the F case was observed whereas only a small increase of the degeneracy of GS was postulated.

The real-space renormalization-group method was applied to the AF Ising model with a transverse field on a triangular lattice.[6] We have found that the "frustrated" Wannier state[19] persists up to the critical ratio $(h/J)_c \approx 1.41$, which is itself considerably reduced from its conjectured value $(h/J)_c \approx 5$ for the F case.[3]

In another study,[7] we have investigated the stability of the "frustrated" Wannier state with respect to quantum tunneling represented by a XY-like term. We have observed an extreme sensitivity of the Wannier state: it is unstable even for infinitesimal tunneling.

In this paper we present the renormalization-group (RG) calculations of a $s=\frac{1}{2}$ XY-like model with a z field which allows a continuous interpolation between F and AF situations. The studies were made on triangular and square lattices. The critical fields were calculated exactly. The RG method was used to recalculate the critical fields and for evaluation of the ground-state energy as well as of critical behavior. We observed the characteristic features of quantum frustration as the increase of the GS energy and the reduction of critical fields. The scaling properties of F and AF (frustrated case) turned out to be very different.

The paper is organized as follows: in Sec. II we define the model: in Sec. III the exact values of critical field are derived; in Sec. IV the RG recursion relations are derived and used to describe the scaling properties, the correlation functions, and the GS energy; and in Sec. V we present the discussions and conclusions. Several technical aspects of calculations are illustrated in the Appendix. Some of the presented results concerning the triangular lattice were announced already in letter form.[8]

II. DESCRIPTION OF THE MODEL

Consider a classical planar interaction between neighboring unit-vector spins at sites i and j of a regular lattice in the form

$$H_c=-\frac{J}{2}\sum_{\langle ij\rangle}\cos[\theta-(\phi_i-\phi_j)],\quad J>0\ , \tag{1}$$

where ϕ_i-ϕ_j is an angle between neighboring spins and θ is a parameter. Quantum extention of (1) can be obtained by expanding cos in (1) and associating the $s=\frac{1}{2}$ spin operators $(S_i^xS_j^x+S_i^yS_j^y)$ and $(S_i^xS_j^y-S_i^yS_j^x)$ with $\cos(\phi_i-\phi_j)$ and $\sin(\phi_i-\phi_j)$, respectively. Thus

$$H'=-\frac{J}{2}\sum_{\langle ij\rangle}[\cos\theta(S_i^xS_j^x+S_i^yS_j^y)+\sin\theta(S_i^xS_j^y-S_i^yS_j^x)] \tag{2}$$

results, with

$$S^x=\begin{pmatrix}0&1\\1&0\end{pmatrix}\ ,$$

etc., and $J>0$.

The antisymmetric part of (2) can be rewritten as $\sum_{\langle ij\rangle}\vec{D}_{ij}\cdot\vec{S}_i\times\vec{S}_j$, where $\vec{D}_{ij}=(0,0,-J/2\sin\theta)$ is the Dzialoshinsky-Moriya (DM) antisymmetric $(\vec{D}_{ij}=-\vec{D}_{ji})$ exchange. The condition $\vec{D}_{ij}=-\vec{D}_{ji}$ amounts to introducing an orientation of bonds $\langle ij\rangle$ in order to define unambiguously the sign of interactions. Using $\epsilon_{ij}=\pm1$ and adding a transverse field to (2) we obtain

$$H=H'-h\sum_l S_l^z=-J\sum_{\langle kl\rangle}[\cos\theta(S_k^+S_l^-+S_k^-S_l^+)+i\sin\theta\epsilon_{kl}(S_k^+S_l^--S_k^-S_l^+)]-h\sum_i S_i^z,\quad h>0\ . \tag{3}$$

The possible choice of signs ϵ_{ij} for a given lattice is a matter of convention and depends on lattice geometry. Eq. (3) together with a sign convention defines a model in question. The sign convention can be also seen as a given distribution of orientations of $\vec{D}_{ij}$. In other words (3) is a quantum spin model coupled to a classical vector field on a lattice.

The Hamiltonian (3) includes as special cases the ferromagnetic (F) XY $(\theta=0)$ and antiferromagnetic (AF) XY $(\theta=\pi)$ models. For $\theta=\pi/2$ it becomes the DM model. On bipartite lattices (3) is equivalent to the F XY model; it can be seen by rotating all the spins of *one* sublattice by θ. Therefore it is particularly interesting to study (3) on nonbipartite lattices, on which already classical AF Ising model shows a frustrated behavior. The purely F case of (3) is the only situation for which a limited number of exact results exists.[26] This case was considered in much detail recently.[4] For either of $\theta\neq0$ case of (3) on nonbipartite lattices or for (3) on oriented square lattice (see below) no exact results were known until now. In particular, it is not known

whether the ground state of (3) is degenerate. It is believed, however, that even if the degeneracy does exist it is not large.[27] Also (3) has a continuous spectrum up to $(h/J)_c(\theta)$, where the gap between the singlet ground state and a band of excited states opens. It is expected that for $\theta \neq 0$ the gap opening occurs for lower fields than for $\theta = 0$, nonfrustrated case. Furthermore the difference between the $\theta = 0$ and $\theta \neq 0$ cases should be more pronounced near $h = 0$ than near $h = h_c$ because the transverse field should mask the frustration effect. These expectations are confirmed by the results of following sections.

Let us consider the orientation conventions in more detail. For the triangular lattice the choice of coordinate axis and the bond orientation is illustrated in Fig. 1, together with the $n_s = 7$ spin block used for the RG calculation. It can be seen that the choice of positive orientation of all the bonds is compatible with the symmetry of the lattice. The field of vectors $\vec{D}_{ij}$ can be best illustrated by forming a lattice out of centers of bonds on the triangular lattice. This kind of a bond lattice is the Kagomé lattice with every point having positive orientation. For the square lattice two orientation choices are possible. The corresponding bond lattice is also a square lattice and the fields of vectors $\vec{D}_{ij}$ can be easily seen. These two choices, rows of alternating in sign $\vec{D}_{ij}$'s and $\vec{D}_{ij} = \text{const} > 0$ everywhere, are equally well compatible with the symmetry of the underlying lattice.

It can be seen by inspection that for another two-dimensional (2D) bipartite lattice—the hexagonal lattice, only one choice of orientations is compatible with its symmetry.

Having introduced the orientations, the models are fully defined. For the nonoriented square lattice, the physical properties should not depend on θ: by rotating the spins of one sublattice by θ in the XY plane the model transforms into ferromagnetic XY. In contrast, for the model of Fig. 1 (model T) there are three sublattices; in the model of Fig. 2 (model S) the local orientations of two sublattices A and B are different. We expect therefore that their physical properties will depend on θ.

Before presenting the details of the calculations let us note that the global properties of the ground state show some periodicity as a function of θ. The period can be obtained from the symmetry considerations. For the model T let us perform the following gauge transformation: rotate the spins in the XY plane on the sublattice A by O, on the sublattice B by $2\pi/3$, and on the sublattice C by $-2\pi/3$. The Hamiltonian transforms itself $H(\theta) \rightarrow H(\theta + 2\pi/3)$. The intrinsic periodicity is therefore $2\pi/3$. If we now consider the elementary triangular plaquette of the triangular lattice, we see that if by going around it we increase the angle θ by $\pi/3$, we arrive at $\theta = \pi$ (AF coupling) after one "tour." Therefore $\theta = \pi/3$ corresponds to the frustrated AF situation. For the model S we label the rows (or columns) by p and we consider an

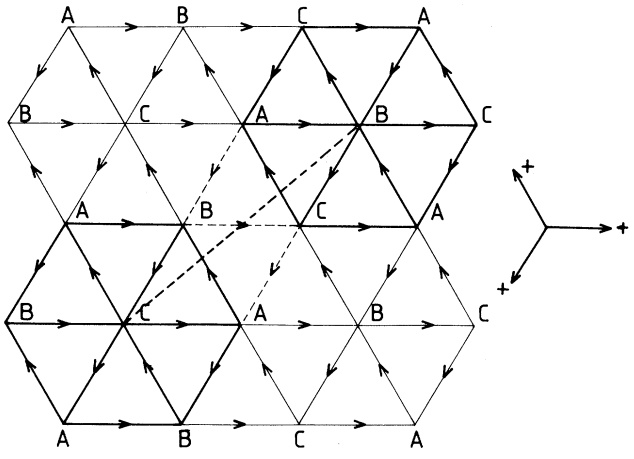

FIG. 1. Choice of the coordinate axes and the orientation convention (the arrows) for the model of Eq. (3) on a triangular lattice, model T. The hexagonal blocks ($n_s = 7$) are coupled through the superbond (dashed line) which has always a positive orientation. Three sublattices of a triangular lattice are represented by A, B, and C. The bonds out of any point on *any* sublattices have the same, positive orientations.

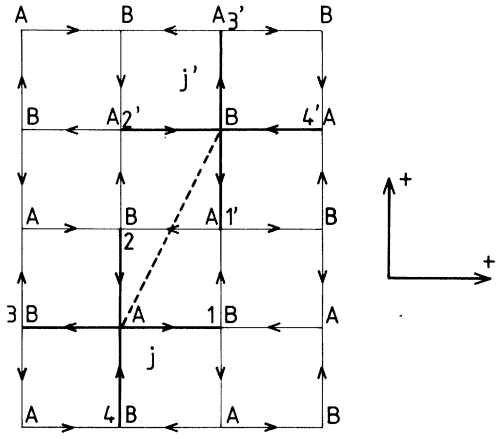

FIG. 2. Choice of the coordinate axes and the orientation convention (the arrows) for the model of Eq. (3) on a square lattice, model S. Two cross-shaped blocks, j and j' ($n_s = 5$) are coupled through the superbond (dashed line) which has a negative orientation because it cuts through a negative bond of the original lattice. The orientations around any point on the sublattice A are opposite to the orientations of bonds out of any point of B sublattice. This renders the two sublattices inequivalent. The numbering of spins in the blocks corresponds to a fixed phase of the wave functions on both blocks j and j'.

elementary square plaquette. By rotating the spins on A sublattice by $\{[1+(-1)^p]/2\}\pi$ and on B sublattice by $\{[2+(-1)^p]/2\}\pi$ we get $H(\theta)\rightarrow H[\theta+(\pi/2)]$, i.e., the periodicity $\pi/2$. By increasing the angle by $\pi/4$ after one "tour" we arrive at π (AF coupling). The above periodicities and values of AF couplings are confirmed by the subsequent calculations.

III. CRITICAL FIELDS

The critical ratio $(h/J)_c$ divides two $T=0$ phases of the model: below $(h/J)_c$ there is no gap between the (unknown) ground state and the continuum of excited states. At $(h/J)_c$ a gap opens. Since $[H, \sum_i^N S_i^z]=0$ the energy spectrum can be conveniently classified in terms of eigenstates of $\Sigma^z=\sum_i^N S_i^z$: $N, N-2, N-4 \ldots, -(N-2), -N$. Above $(h/J)_c$ the ground state is singlet and corresponds to all the spins pointing in the z direction and its ground-state energy is $E_N=-Nh$. The first excited state is the ground state of the sector $\Sigma^z=N-2$ and has the energy $E_{N-2}=e_{N-2}J-(N-2)h$, where e_{N-2} is the ground-state energy of $(1/J)H'$ in the sector $\Sigma^z=N-2$. Consequently the energy gap above the $(h/J)_c$ is equal to $\Delta=2h+Je_{N-2}$. The gap is vanishing at the critical ratio

$$\left(\frac{h}{J}\right)_c=-\frac{e_{N-2}}{2} \quad . \tag{4}$$

To find e_{N-2} for a particular model consider first a wave function $\phi_{m,n}$ describing all the spins pointing in z direction except if a spin at row m and column n is pointing in the $-z$ direction. It satisfies

$$\frac{1}{J}H'\phi_{m,n}=-\cos\theta\sum_{\delta(m,n)}\phi_{\delta(m,n)} - i\sin\theta\sum_{\delta(m,n)}\epsilon(\delta(m,n))\phi_{\delta(m,n)} \quad . \tag{5}$$

Here $\delta(m,n)$ denotes a nearest neighbor of (m,n) and $\epsilon(\delta(m,n))$ denotes an orientation of a bond between (m,n) and its nearest neighbor $\delta(m,n)$. The complete ground-state function of the $\Sigma^z=N-2$ sector is a linear combination

$$\Phi_{N-2}=\sum_{\text{all } m,n}a_{m,n}\phi_{m,n} \quad , \tag{6}$$

and satisfies

$$\frac{1}{J}H'\Phi_{N-2}=E_{N-2}\Phi_{N-2} \quad . \tag{7}$$

Using Eqs. (5), (6), and (7) the following equation determines e_{N-2}:

$$e_{N-2}a_{m,n}=\cos\theta\sum_{\delta(m,n)}a_{\delta(m,n)} + i\sin\theta\sum_{\delta(m,n)}\epsilon(\delta(m,n))a_{\delta(m,n)} \quad . \tag{8}$$

There again $\delta(m,n)$ denotes a nearest neighbor of (m,n). Eq. (8) applies only to a system for which orientations around different sublattices are the same, for instance model T. For model S the orientations around a point of A sublattice and B sublattice are different and Φ_{N-2} can be conveniently represented as

$$\Phi_{N-2}=\sum_{\text{all } m,n\in A}a_{m,n}\phi_{m,n}+\sum_{\text{all } i,j\in B}b_{i,j}\psi_{i,j} \quad , \tag{9}$$

where now $\psi_{i,j}$ is an equivalent of $\phi_{m,n}$ but on the B sublattice. Using Eq. (7) one obtains a set of coupled equations

$$e_{N-2}a_{m,n}=-\cos\theta\sum_{\delta(m,n)}b_{\delta(m,n)}+i\sin\theta\sum_{\delta(m,n)}\epsilon(\delta(m,n))b_{\delta(m,n)} \quad , \tag{10a}$$

$$e_{N-2}b_{m,n}=-\cos\theta\sum_{\delta(m,n)}a_{\delta(m,n)}-i\sin\theta\sum_{\delta(m,n)}\epsilon(\delta(m,))a_{\delta(m,n)} \quad . \tag{10b}$$

Equations (8), (10a), and (10b) can be solved by means of Fourier transformation.

A. Model T

The orientations of the axes of the point (m,n) are illustrated in Fig. 3. The function $\Phi_{m,n}$ satisfies

$$\frac{1}{J}H'\phi_{m,n}=-[\cos\theta(\phi_{m+1,n}+\phi_{m-1,n}+\phi_{m,n+1}+\phi_{m,n-1}+\phi_{m+1,n+1}+\phi_{m-1,n-1}) + i\sin\theta(\phi_{m+1,n}-\phi_{m-1,n}+\phi_{m,n+1}-\phi_{m,n-1}+\phi_{m+1,n+1}-\phi_{m-1,n-1})] \quad , \tag{11}$$

and the coefficients $a_{m,n}$ satisfy

$$e_{N-2}a_{m,n}=-[\cos\theta(a_{m+1,n}+a_{m-1,n}+a_{m,n+1}+a_{m,n-1}+a_{m+1,n+1}+a_{m-1,n-1}) - i\sin\theta(a_{m+1,n}-a_{m-1,n}+a_{m,n+1}-a_{m,n-1}+a_{m+1,n+1}-a_{m-1,n-1})] \quad . \tag{12}$$

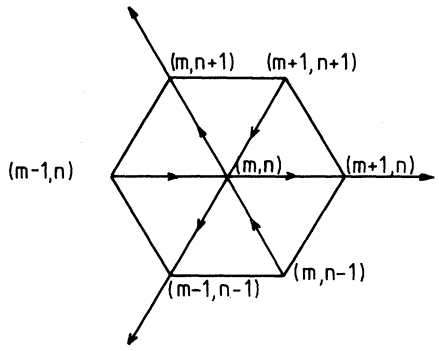

FIG. 3. The numbering of spins for a hexagonal block used to calculate the critical field.

We introduce now a parallelogram of $N=N_1N_2$ atoms with N_1 rows and N_2 columns. Now

$$a_{m,n}=\frac{1}{N}\sum_{k,l}a_{k,l}\exp i(K_k m+K_l n) \ , \tag{13}$$

where $K_k=\pi k/N_1$, $K_l=\pi l/N_2$ and

$$k,l=-N_{1,2},\ -N_{1,2}+1,\ \ldots\ N_{1,2}-1 \ .$$

We obtain

$$e_{N-2}(K_k,K_l,\theta)=-2\{\cos(\theta-K_k)+\cos(\theta-K_l)+\cos[\theta-(K_k+K_l)]\} \ . \tag{14}$$

The minima of $e_{N-2}(K_k,K_l)$ appear at

$$K_k=K_l=\frac{2\theta}{3}+\frac{2n\pi}{3}, \quad n=0,1,2,\ \ldots \ .$$

Using Eq. (4) we obtain the critical field

$$\left[\frac{h}{J}\right]_c(\theta)=3\cos\left[\theta-\frac{n2\pi}{3}\right], \quad n=0,1,2,3\ \ldots \tag{15}$$

for $(2n-1)(\pi/3)<\theta<(2n+1)(\pi/3)$; for $\theta=0$ [mod $(2\pi/3)$], ferromagnetic case, we recover the exact result[28] $(h/J)_c=3$. We observe that $(h/J)_c(\mathrm{AF})=0.5(h/J)_c(\mathrm{F})$.

B. Model *S*

The orientation of the axes of the point (m,n) are illustrated in Fig. 2. The functions ϕ and ψ satisfy

$$\frac{1}{J}H'\phi_{m,n}=e_{N-2}\phi_{m,n}=-[\cos\theta(\psi_{m+1,n}+\psi_{m-1,n}+\psi_{m,n+1}+\psi_{m,n-1})+i\sin\theta(-\psi_{m+1,n}-\psi_{m-1,n}+\psi_{m,n+1}+\psi_{m,n+1})] \tag{16a}$$

and

$$\frac{1}{J}H'\psi_{m,n}=e_{N-2}\phi_{m,n}=-[\cos\theta(\phi_{m+1,n}+\phi_{m-1,n}+\phi_{m,n+1}+\phi_{m,n-1})-i\sin\theta(-\phi_{m+1,n}-\phi_{m-1,n}+\phi_{m,n+1}+\phi_{m,n-1})] \ . \tag{16b}$$

The coefficients $a_{m,n}$ and $b_{m,n}$ of Eq. (9) satisfy now [see Eq. (10)] the coupled equations

$$e_{N-2}a_{m,n}=-\cos\theta(b_{m+1,n}+b_{m-1,n}+b_{m,n+1}+b_{m,n-1})-i\sin\theta(-b_{m+1,n}-b_{m-1,n}+b_{m,n+1}+b_{m,n-1}) \ , \tag{17a}$$

$$e_{N-2}b_{m,n}=-\cos\theta(a_{m+1,n}+a_{m-1,n}+a_{m,n+1}+a_{m,n-1})-i\sin\theta(-a_{m+1,n}-a_{m-1,n}+a_{m,n+1}+a_{m,n-1}) \ . \tag{17b}$$

Again after Fourier transforming and solving for $e_{N-2}(K_l,K_m)$ [compare Eq. (13)] we obtain

$$e^2_{N-2}(K_l,K_m,\theta)=4(\cos^2 2K_l+\cos^2 2K_m+2\cos 2\theta\cos 2K_l\cos 2K_m) \ . \tag{18}$$

By minimizing with respect to K_l and K_m, we get $e_{N-2}(\theta)=-4\cos\theta$. Upon utilizing Eq. (4) we obtain

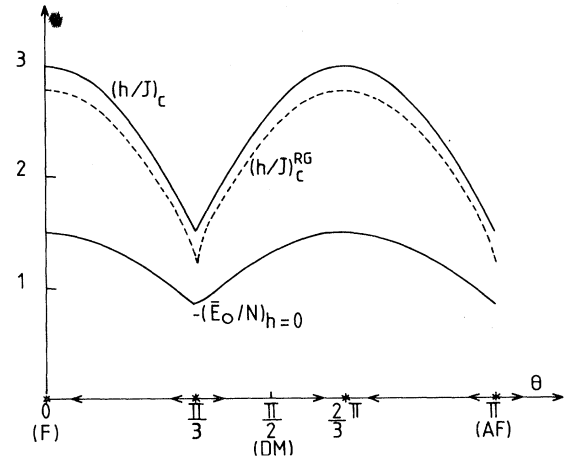

FIG. 4. Model *T*. Exact results for the critical field (full upper curve) and renormalization-group results for the critical field (dashed upper curve) and for the GS energy per site.

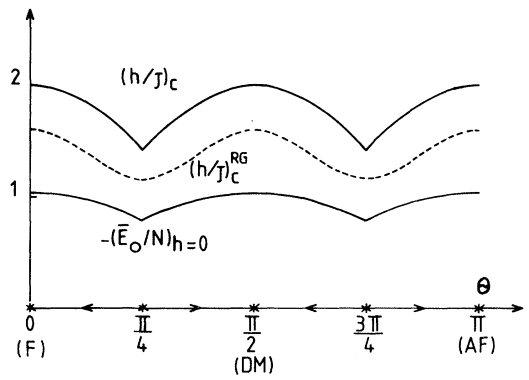

FIG. 5. Model S. Exact results for the critical field (full upper curve) and renormalization-group results for the critical field (dashed upper curve) and for the GS energy per site.

finally the exact expression for the depression of the critical field with θ

$$\left(\frac{h}{J}\right)_c(\theta)=2\cos\left(\theta-n\frac{\pi}{2}\right) \tag{19}$$

for $(2n-1)(\pi/4)<\theta<(2n+1)(\pi/4), n=0,1,2,\ldots$.

For $\theta=0(\mathrm{mod}\,\pi/2)$ which is the F case we again recover the exact result.[28] We note that contrary to the T model, the pure DM interaction ($\theta=\pi/2$) does not lead here to any reduction of critical field. This is due to the invariance of Eq. (19) under rotation by $\pi/2$. Equations (15) and (19) are plotted in Figs. 4 and 5.

IV. RENORMALIZATION-GROUP RECURSION RELATIONS

In this section we shall present the formulation of the real-space renormalization group as applied to the generalized $s=\frac{1}{2}XY$ model of Eq. (3). The application of this method to the pure XY model with the external field in the z direction was already discussed for the 1D case in Ref. 2 and for the 2D case in Refs. 4 and 5. We shall adopt the same notation as in Ref. 4. Since as in the previous studies here also $[H,\sum_i S_i^z]=0$, the energy eigenvalues of H will be classified according to the eigenvalues of $\Sigma^z\equiv\sum_i S_i^z$. We suppose that at the nth iteration the Hamiltonian can be written in the form

$$H^{(n)}=-\frac{1}{2}J^{(n)}\sum_{\langle kl\rangle}[\cos\theta^{(n)}(S_k^{x(n)}S_l^{x(n)}+S_k^{y(n)}S_l^{y(n)})+i\sin\theta^{(n)}\epsilon_{kl}^{(n)}(S_k^{x(n)}S_l^{y(n)}-S_k^{y(n)}S_l^{x(n)}]$$
$$-h^{(n)}\sum_k S_k^{z(n)}+C^{(n)}\sum_k I_k^{(n)}\ , \tag{20}$$

where $\langle kl\rangle$ represents a pair of nearest neighbors, $I_k^{(n)}$ is the unit matrix at site k, the initial values of $J^{(n)}$, $h^{(n)}$ and $C^{(n)}$ being

$$J^{(0)}=J,\quad h^{(0)}=h,\quad C^{(0)}=0\ , \tag{21}$$

and the set $\{\epsilon_{kl}^{(n)}\}$, ($\epsilon_{kl}^{(n)}=\pm1$) defines the orientations of nearest-neighbor (NN) bonds. The initial choice $\{\epsilon_{kl}^{(0)}\}$ is a matter of convention and, in fact, defines the model (see the above discussion).

We now group the neighboring spins into the spin blocks of n_s sites and rewrite $H^{(n)}$ as a sum of single-block Hamiltonian $H_j^{(n)}$ and the terms describing the interactions between the neighboring blocks j,j', $H_{j,j'}^{(n)}$:

$$H^{(n)}=\sum_j\left(H_j^{(n)}+C^{(n)}\sum_{p=1}^{n_s}I_{j,p}^{(n)}\right)+\sum_{\langle j,j'\rangle}H_{j,j'}^{(n)}\ , \tag{22}$$

where

$$H_j^{(n)}=-\tfrac{1}{2}J^{(n)}\sum_{\langle p,p'\rangle}[\cos\theta^{(n)}(S_{j,p}^{x(n)}S_{j,p'}^{x(n)}+S_{j,p}^{y(n)}S_{j,p'}^{y(n)})+i\sin\theta^{(n)}\epsilon_{pp'}^{(n)}(S_{j,p}^{x(n)}S_{j,p'}^{y(n)}-S_{j,p}^{y(n)}S_{j,p'}^{x(n)})]-h^{(n)}\sum_{p=1}^{n_s}S_{j,p}^{z(n)}\ , \tag{23}$$

and

$$H_{j,j'}^{(n)}=-\tfrac{1}{2}J^{(n)}\sum_{\substack{p,p'\\ \langle j,p,j',p'\rangle}}[\cos\theta^{(n)}(S_{j,p}^{x(n)}S_{j',p'}^{x(n)}+S_{j,p}^{y(n)}S_{j',p'}^{y(n)})+i\sin\theta^{(n)}\epsilon_{p,p'}^{(n)}(S_{j,p}^{x(n)}S_{j',p'}^{y(n)}-S_{j,p}^{y(n)}S_{j',p'}^{x(n)})]\ . \tag{24}$$

In the last expression $\langle j,p;j',p' \rangle$ is a NN pair where $p(p')$ belongs to $j(j')$ block.

The first step in the RG procedure is to diagonalize exactly the single-block Hamiltonian $H_j^{(n)}$. The two lowest-lying energy states of a block are retained. They form a new truncated basis in which the new parameters of the system are recalculated by evaluation of the matrix elements of $H_{j,j'}^{(n)}$. The whole procedure is repeated until no changes of parameters are observed (fixed point). The unstable fixed points of the RG transformation usually signal the onset of the phase transition in the ground state. We diagonalize $H_j^{(n)}$ in the basis of eigenvectors of $\Sigma_j^{z(n)}$ in the form $|\delta_1, \delta_2, \ldots \delta_{n_s}\rangle$ where $\delta_p = \pm 1$ is the eigenvalue of the zth component of pth spin in the block. On this basis $H_j^{(n)}$ will decouple into block-matrix form with n_s blocks numbered by q ($q = 1, 2, \ldots n_s$). The block matrices are the representations of $H_j^{(n)}$ in the subspaces q corresponding to a given eigenvalues $(-n_s + 2q - 2)$ of $\Sigma_j^{(n)}$. If we denote by $|q\rangle$ the ground-state wave function of $H_j^{(n)}$ in the subspace q, then its energy is

$$E_q^{(n)} = (n_s - 2q + 2)h^{(n)} + e_q^{(n)} J^{(n)}, \qquad q = 1, \ldots n_s \ , \tag{25}$$

where $e_q^{(n)}$ is the lowest eigenvalue of

$$\left(J^{(n)}\right)^{-1}\left[H_j^{(n)} + h^{(n)} \sum_{p=1}^{n_s} S_{j,p}^{z(n)}\right] .$$

As in Refs. 4 and 5 for a given $h^{(n)}/J^{(n)}$ the two lowest-lying states of $H_j^{(n)}$ are always the ground states of adjacent subspaces q and $q+1$. The block spin $\vec{S}_j$ can be now introduced by rewriting $H_j^{(n)}$ as

$$\begin{aligned} H_j^{(n)} &= \tfrac{1}{2}(E_q^{(n+1)} - E_{q+1}^{(n+1)}) S_j^{z(n+1)} \\ &\quad + \tfrac{1}{2}(E_q^{(n+1)} + E_{q+1}^{(n+1)}) I_j^{(n+1)} \\ &\equiv -h^{(n+1)} S_j^{z(n+1)} + C^{(n+1)} I_j^{(n+1)} \ , \end{aligned} \tag{26}$$

where, using Eq. (25)

$$h^{(n+1)} = h^{(n)} + \tfrac{1}{2}(e_q - e_{q+1}) J^{(n)} \ . \tag{27}$$

In Eqs. (26) and (27) we have identified $|q\rangle$ and $|q+1\rangle$ with the "down" and "up" eigenstates of $S_j^{z(n+1)}$ called $|\mp\rangle^{(n+1)}$, respectively.

In order to calculate the recursion relation between the coupling constants we have to calculate the recursion relations between the spin components. If, as before, p denotes the position of spin within the block, by calculating the matrix elements of $\vec{S}_{j,p}^{(n)}$ for given q we get

$$S_{j,p}^{\pm(n)} = \xi_{pq}^{\pm} S_j^{\pm(n+1)} \quad [\xi_{pq}^{\pm} = \xi_{pq}^{\pm}(\theta)] \ , \tag{28}$$

where, depending on p and q, $\xi_{pq}^{+} = \xi_{pq}^{-}$ or $\xi_{pq}^{+} = (\xi_{pq}^{-})^*$. With relations (28) the matrix elements of $H_{j,j'}^{(n)}$ can be evaluated and can be written for a given q as

$$\langle + | H_{j'j}^{(n)} | - \rangle_q = -J^{(n)} \cos\theta^{(n)} K_q(\theta^{(n)}) - iJ^{(n)} \sin\theta^{(n)} L_q(\theta^{(n)}) \ , \tag{29}$$

with K_q and L_q functions of $\xi_{pq}^{\pm}$ and of orientations $\{\epsilon_{kl}\}$. Consequently the new coupling $J^{(n+1)}$ and the new angle $\theta^{(n+1)}$ can be defined by

$$\begin{aligned} &-J^{(n)} \cos\theta^{(n)} K_q(\theta^{(n)}, \{\epsilon_{kl}^{(n)}\}) \\ &\quad - iJ^{(n)} \sin\theta^{(n)} L_q(\theta^{(n)}, \{\epsilon_{kl}^{(n)}\}) \\ &\qquad \equiv -J^{(n+1)} \cos\theta^{(n+1)} - iJ^{(n+1)} \sin\theta^{(n+1)} \ . \end{aligned} \tag{30}$$

From (30) the recursion relations read

$$\tan\theta^{(n+1)} = \frac{L_q(\theta^{(n)})}{K_q(\theta^{(n)})} \tan\theta^{(n)} \ , \tag{31}$$

and

$$\begin{aligned} J^{(n+1)} &= J^{(n)} [\cos^2\theta^{(n)} K_q^2(\theta^{(n)}) \\ &\qquad + \sin^2\theta^{(n)} L_q^2(\theta^{(n)})]^{1/2} \\ &\equiv J^{(n)} N(\theta^{(n)}) \ . \end{aligned} \tag{32}$$

Equations (27), (31), and (32) define the new coupling constants in terms of old coupling constants and the old orientations. For the two choices of orientations of triangular and square lattice (Figs. 1 and 2) which led to the reduction of critical fields [Eqs. (15) and (19)] the new orientations $\{\epsilon_{kl}^{(n+1)}\}$ can be unambiguously defined by the following convention: the orientation of the superbond between the superblocks at stage $(n+1)$ is the orientation of that bond at stage (n) which was cut by this superbond. It can be readily seen from Figs. 1 and 2 that with this convention the resulting lattice of superblocks has the same set of orientations as the initial lattice.

By analyzing the recursion relations for different q we have encountered the problem which has been already discussed at length in Ref. 4; only the recursion relations $q = n_s$, $q = 1$ and if n_s is odd, $q = q_0 = (n_x + 1)/2$ give the physical fixed points. Other fixed points lie always outside the zones of validity of recursion relations. Therefore we had limited ourselves here to only two limiting cases: $q = n_s$, which describes the region near $(h/J)_c$, and $q = q_0$, which describes the region $(h/J) \sim 0$. (From now on we drop the index q.) Similarly to the pure XY model, the analysis of the recursion relations did not lead to any ordering. This means that within the two-level approximation there is no spontaneous magnetization in the system. We do not claim this result to be exact, but we just mention that if it is not proven that $\theta = 0$ (F case) orders, it is even less likely that $\theta \neq 0$ model orders because of the destructive

TABLE I. Model T. Exact and RG results for the location of the critical field and the RG results for the critical exponents and the ground-state energy per spin in the two [F($\theta=0$) and AF($\theta=\pi$)] cases.

θ	$(h/J)_c$ Exact	$(h/J)_c$ RG	$(-\bar{E}/N)_{h=0}$ RG	$h=0$ z	$h=0$ η	$h=h_c$ z_c	$h=h_c$ 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

effect of frustration on ordering. The finite-cell calculation indicates some degree of ordering,[27] but it would be highly desirable to have some exact results. A good test of the RG mehtod is to calculate the critical fields $(h/J)_c(\theta)$ using the two-level scheme. The calculations are done along the lines indicated above using the recursion relations $q=n_s$ and $q=n_s-1$. The results for the hexagon and the cross are presented in the Figs. 4 and 5. In the case of the cross an analytical calculation is possible. It has been reproduced in the Appendix.

Since no magnetization was detected it has been assumed as a working hypothesis that the correlation function, i.e., $\rho_x(R)=\langle 0|S_0^x S_R^x|0\rangle$ have the power-law behavior,

$$\rho_x(R) \underset{R\to\infty}{\to} R^{-\eta_x} .$$

In order to avoid the edge effects, the block-averaged quantities were renormalized,

$$\sigma^x=\frac{1}{n_s}\sum_{p=1}^{n_s} S_p^x ,$$

by introducing the averaged ξ's by

$$\bar{\xi}=(n_s)^{-1}\sum_{p=0}^{n_s}\xi_p \quad [\bar{\xi}=\bar{\xi}(\theta)] .$$

Using now that in units of lattice spacing $R=n_s^{n/2}$ and $\langle 0|\sigma_0^x\sigma_R^x|0\rangle \underset{n\to\infty}{\to} (\bar{\xi})^{2n}$ we obtain directly ($\eta=\eta_x$)

$$\eta=-4\frac{\ln\bar{\xi}}{\ln n_s} . \tag{34}$$

Similarily the dynamical exponent z which tells how the energy renormalizes with the change of scale at the fixed point can be directly extracted from (32):

$$J^{(n+1)}=(n_s)^{-1/2z}J^{(n)} \tag{35}$$

and

$$z=-2\frac{\ln N(\theta)}{\ln n_s} .$$

The results for η and z can be in principle obtained in two limits, $(h/J)\approx 0$ and $(h/J)\approx(h/J)_c$. In the former limit the calculations can be reduced to the diagonalization of 5×5 (model S) and 10×10 (model T) matrices, respectively. In the latter limit for the model S the analytical calculations are reproduced in the Appendix. For the both models $\theta=0$ (F case) was found to be the stable fixed point. $\theta_{c1}=(\pi/3)\times[\mathrm{mod}(2\pi/3)]$ and $\theta_{c2}=(\pi/4)[\mathrm{mod}(\pi/2)]$ correspond to the AF situation for models T and S, respectively, and were found to be the unstable fixed points.

Hence the critical behavior at any θ except θ_{c1} (θ_{c2}), [models $T(S)$] is *identical* to that of $\theta=0$ case. The values of exponents are presented in the Tables I and II. Notice there is a distinct increase of both z

TABLE II. Model S. Exact and RG results for the location of the critical field and the RG results for the critical exponents and the ground-state energy per spin in the two [F($\theta=0$ and AF($\theta=\pi$)] cases.

θ	$(h/J)_c$ Exact	$(h/J)_c$ RG	$(-\bar{E}/N)_{h=0}$ RG	$h=h_c$ z_c	$h=h_c$ η_c
0(F)	2	1.6	1.03	1.22	2.13
π(AF)	1.41	1.14	0.79	2.58	2.67

and η by going from the F to AF situations which reflects different scaling properties of the AF case.

The ground state energy E_0/N for $h=0$, (n_s odd as the cases here) can be evaluated by cumulating the constant terms $C^{(n)}$ appearing in Eq. (26). Because of important shape and edge effects in 2D, the resulting summation has to be appropriately weighted. A possible approach was described in Sec. V of Ref. 4, where it has been shown that the upper and lower bounds for E_0/N can be estimated by summing $C^{(n)}$ averaged over the number of sites and bonds, respectively. It has been shown[4] that the arithmetical average between these two estimates gives generally satisfactory results when compared with other existing estimates. We used Eqs. (29) and (31) of Ref. 4 to evaluate $E_0(\theta)/N$. The results are presented in Figs. 4 and 5. A clear reduction of the absolute value of E_0/N for $\theta=\theta_{c_1}$, θ_{c_2} can be seen; it corresponds to the fact that the frustrated case is energetically less stable that the F case. For the T model the value of $E_0(\pi)$ of Ref. 27 is well reproduced.

V. DISCUSSION AND CONCLUSION

The treatment of the GS of the generalized $s=\frac{1}{2}$ XY model [Eq. (3)] on the nonbipartite lattices—triangular and square with nonequivalent sublattices—revealed some new properties of the quantum AF case. First of all the frustrated AF case was found to be very unstable; it is described by the unstable fixed point. Its GS energy is increased as compared to the F case although the increase is smaller than in the classical (Wannier) model. The reduction of critical fields in the AF case means that it is easier to open a gap—a fact which is consistent with the increase of the GS energy. The behavior of the correlation functions differs also from the F case. If we accept the hypothesis about the power-law behavior of the correlations functions (its validity may be questioned[29]) then the η and z in AF case are larger than in the F case for both $h=0$ and $h=h_c$. It means that the tendency to order (if order exists at all) is clearly reduced in the frustrated case. This is also reminiscent of the Wannier state without ordering.

The classical $s=\infty$ AF XY was also investigated[30]; here also the GS energy is raised, the nature of the GS is more complicated than in the F case while the DM model maps onto the F situation as in the quantum model T above.

This RG study may be extended to other spin systems like the $s=\frac{1}{2}$ AF Heisenberg model on the triangular lattice as well as to impure and disordered frustrated systems. Similar effects are also expected to occur in the fermion systems. In particular the ground-state properties of vacancies on the triangular lattice are of considerable interest in explaining the behavior of ^{3}He in confined geometries.[31,32] As a starting point one uses usually some sort of hopping Hamiltonian (tightly bound fermions). Even without the interactions the triangular lattice has an important effect on magnetic properties. Interestingly enough the spectrum of the vacancy band on the triangular lattice is identical to our expression for $e_{N-2}(K_1,K_2)$, Eq. (14). The dissymmetry of vacancy band is the source of specific properties of ^{3}He. Another way for "frustrating" the quantum systems was suggested very recently,[33] using powerful diagonalization procedures. The effect of introducing a finite number of odd rings in a structure of otherwise even rings was shown to produce a change in the band edge. Here also only a noninteracting hopping Hamiltonian was used. The moving of the band edge is again equivalent to the changes in $(h/J)_c$ in 2D spin models.

It would be interesting to investigate the effects of interactions on such structures with and without defects.

Also it would be highly desirable to develop a unified method to treat the frustrated spin and fermion systems.

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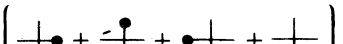
APPENDIX A: RENORMALIZATION-GROUP CALCULATION OF THE CRITICAL FIELDS AND THE SCALING PROPERTIES NEAR THE CRITICAL FIELDS ON THE SQUARE LATTICE

We will present here as an example the RG calculations of $(h/J)_c(\theta)$ and the scaling properties near $(h/J)_c(\theta)$. The critical field is defined as a point where the gap opens between the ground state with all the spins parallel to z axis and the excited state with one spin deviation. If we use the cross-shaped block with $n_s=5$ we have to diagonalize H in two subspaces $\Sigma^z=5$ and $\Sigma^z=3$. The F (AF) ground state of H in $\Sigma^z=3$ contains the bonding (antibonding) eigenfunction of H, i.e., satisfying $R(\frac{1}{2}\pi)\phi=\pm\phi$, where $R(\alpha)$ is a rotation by α in the plane XY. For general θ it is necessary to look for a linear

combination. If a point denotes $\delta_z=-1$ and

$\phi_0=$  $\equiv|+\rangle$,

$\phi_1=$  ,

$\phi_2=\frac{1}{2}\Big($  $\Big)$, (A1)

$\phi_3=\frac{1}{2}\Big($  $\Big)$,

then in this basis the block Hamiltonian has the matrix

	ϕ_1	ϕ_2	ϕ_3
ϕ_1	0	$-2J\cos\theta$	$-2iJ\sin\theta$
ϕ_2	$-2J\cos\theta$	0	0
ϕ_3	$+2iJ\sin\theta$	0	0

(A2)

and its ground-state wave function is

$$\phi_G=\frac{1}{\sqrt{2}}\phi_1+\frac{\cos\theta}{\sqrt{2}}\phi_2-\frac{i\sin\theta}{\sqrt{2}}\phi_3\equiv|-\rangle \quad \text{(A3)}$$

with the energy eigenvalue $e_5=-2$. By calculating the matrix elements for the "peripheric" spins $p=1,\ldots 4$, we obtain

$$\xi_{1,3}\equiv\xi_1=\langle\phi_0|S^{\pm}_{1,3}|\phi_G\rangle=\frac{1}{2\sqrt{2}}e^{i\theta} ,$$
$$\xi_{2,4}\equiv\xi_2=\langle\phi_0|S^{\pm}_{2,4}|\phi_G\rangle=\frac{1}{2\sqrt{2}}e^{-i\theta} . \quad \text{(A4)}$$

By evaluating now the interblock coupling using (A4) and the orientation scheme, Fig. 2 the recursion relations take on the form of Eq. (30) with

$$K_5(\theta)=\tfrac{1}{8}(3\cos^2\theta-\sin^2\theta) ,$$
$$L_5(\theta)=\tfrac{1}{8}(\cos^2\theta-3\sin^2\theta) ,$$

and subsequently

$$\tan\theta^{(n+1)}=\frac{3\cos^2\theta^{(n)}-\sin^2\theta^{(n)}}{\cos^2\theta^{(n)}-3\sin^2\theta^{(n)}}\tan\theta^{(n)} . \quad \text{(A5)}$$

One verifies that $\theta=0$ and $\theta=\pi/4$ are stable and unstable fixed point of (A5), respectively.

The new $J^{(n+1)}$ is defined by Eq. (3.2), which reads

$$J^{(n+1)}=J^{(n)}\tfrac{1}{8}M(\theta^{(n)}) , \quad \text{(A6)}$$

where

$$M(\theta)\equiv[16(\cos^6\theta+\sin\theta^6)-8(\cos^4\theta+\sin^4\theta)+1]^{1/2} . \quad \text{(A7)}$$

Together with the new $h^{(n+1)}$ which is now according to (27)

$$h^{(n+1)}=h^{(n)}-J^{(n)} , \quad \text{(A8)}$$

the following relation results for $h^{(n)}/J^{(n)}$:

$$\left(\frac{h}{J}\right)^{(n+1)}=\frac{8}{M(\theta^{(n)})}\left[\left(\frac{h}{J}\right)^{(n)}-1\right] . \quad \text{(A9)}$$

The recursion relation (A10) has the fixed point at the value $(h/J)^*$ which we identify with the approximate critical field[5]

$$\left(\frac{h}{J}\right)_c(\theta)=\frac{8}{8-M(\theta)} . \quad \text{(A10)}$$

By comparing (A10) with the exact result (19) we conclude that (A10) is off by $\sim 20\%$ from the exact value. The exact and approximate relations for $(h/J)_c(\theta)$ are compared in Fig. 5. The dynamical exponent z can be directly obtained from (A6)

$$z=-2\frac{\ln[M(\theta)/8]}{\ln 5} , \quad \text{(A11)}$$

and we get $z(\theta=\pi/4)=2.58$ and $z(\theta=0)=1.22$. The exponent of correlation function is obtained from

$$\eta=-4\frac{\ln\left(\frac{1}{5}\sum_{p=0}^{4}\xi_p\right)}{\ln 5} ,$$

where, if we take into the account that for the "central" spin $\xi_0\equiv\xi_c=1/\sqrt{2}$, we get $\eta(\theta=\pi/4)=2.67$ and $\eta(\theta=0)=2.13$.

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