

Zero-temperature renormalization-group method for quantum systems. IV. $S = \frac{1}{2}XY$ model in a transverse field in two and three dimensions

K. A. Penson, R. Jullien, and P. Pfeuty

Université Paris-Sud, Laboratoire de Physique des Solides, Centre d'Orsay, 91405 Orsay, France*

(Received 27 December 1979)

A zero-temperature real-space renormalization-group method for quantum systems is applied to the $S = \frac{1}{2}XY$ model with a Z field with the Hamiltonian $H = -\frac{1}{2}J \sum_{\langle ij \rangle} [(1+\gamma)S_i^x S_j^x + (1-\gamma)S_i^y S_j^y] - h \sum_i S_i^z$ on quadratic, triangular, and hexagonal lattices in two dimensions (2D) and on a cubic lattice in 3D. In all the isotropic ($\gamma=0$) 2D cases the method gives no order in the ground state $|0\rangle$ but changes in the correlation functions at $(h/J)_c = \frac{1}{2}z'$ [z' is the number of nearest neighbors (NN)] are observed. An argument is presented that at $(h/J)_c$ the method becomes exact in the limit of infinite-size spin blocks. It is suggested that the correlation functions $\langle 0|S_0^\alpha S_R^\alpha|0\rangle$ ($\alpha=x,y$) for large R have a power-law behavior $\sim R^{-\eta}$ for $0 \leq |h/J| < |(h/J)_c|$ with $\eta \approx 1.5$ for $|h/J| < (h/J)_c$ and $\eta = 2$ at $(h/J)_c$. The dynamical exponent z is obtained to be ≈ 0.3 for $|h/J| < \frac{1}{2}z'$ and at $(h/J)_c$ close to 2. An indirect method of calculating the ground-state energy is developed, and the results are compared with the known estimates. For $\gamma \neq 0$ and $h=0$ the γ dependences of the order in the ground state $\mu^x(\gamma)$ is calculated to be $\mu^x \sim \gamma^{0.21}$ for $\gamma \rightarrow 0$ and $h=0$. In a 3D cubic lattice ($\gamma=0$) the analysis of recursion relations indicates the existence of order, in accord with recent exact theorems.

I. INTRODUCTION

The phase transitions in quantum systems have recently been an object of increased theoretical activity. While it is generally believed that the critical behavior of quantum systems at finite temperatures does not very much differ from that of corresponding classical systems, by lowering of temperature there is an increasing interplay between quantum and thermal fluctuations. In the immediate neighborhood of $T=0$ the quantum fluctuations prevail and there is a cross-over to a different critical behavior at precisely $T=0$. In certain cases there exists an exact equivalence between the $T=0$ critical behavior of a D -dimensional quantum system and the $T \neq 0$ critical behavior of corresponding $D+1$ classical system.¹ This is the case of the anisotropic $S = \frac{1}{2}XY$ model with a transverse field. Most of quantum systems have their $T=0$ critical behavior peculiar to their own nature. Not all the details of the critical behavior (critical exponents, etc.) are at present known. This is the situation for instance of the isotropic XY model with a transverse field¹ and with different versions of Hamiltonians with coupled spins and fermions (i.e., Kondo lattice^{2,3}). The exact solutions for quantum spin systems exist only for very specific cases in one dimension (1D).⁴ Therefore there is a need for calculational methods especially suited for quantum systems and not limited to $D=1$.

Recently, a zero-temperature renormalization-group method for quantum systems has been introduced by the field theorists.⁵ This is variational-like, perturbation-theory-free iterative procedure of reconstruction of the ground state $|0\rangle$ of a quantum system and arbitrary expectation values on it. The method was initially applied to several quantum field theory problems.⁵ Subsequently it was extended and critically studied for a large variety of quantum spin systems like a 1D representation of the Kondo-lattice problem,² Ising model with a transverse field in 1D,⁶ on bipartite lattices in 2D,⁷ on the triangular lattice with antiferromagnetic couplings,⁸ and finally on different ramified comblike structures.⁹ Furthermore, the 1D isotropic XY model with a transverse field was examined¹⁰ and the applications to disordered system¹¹ and to the Yang-Lee edge-singularity problem were made.¹² The studies of several other related problems were also undertaken.^{13,14}

In this paper, we shall present the calculation of the critical behavior at $T=0$ of the $S = \frac{1}{2}XY$ model with a transverse field with the Hamiltonian

$$H = -\frac{1}{2}J \sum_{\langle ij \rangle} [(1+\gamma)S_i^x S_j^x + (1-\gamma)S_i^y S_j^y] - h \sum_i S_i^z, \quad (1)$$

with exchange J , the magnetic field h , and the aniso-

tropy γ , and where

$$S_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_i^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

and

$$S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are a set of Pauli matrices on each site, $\langle ij \rangle$ representing a nearest-neighbor pair on a lattice. The case $\gamma \neq 0$ belongs to the universality class $\gamma = 1$ (Ising model¹⁵) and most of the paper will be concerned with the isotropic case, $\gamma = 0$,

$$H = -\frac{1}{2}J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - h \sum_i S_i^z. \quad (2)$$

The information one has about the ground-state properties of Eq. (2) is scarce. The ground-state wave function $|0\rangle$ for $h \rightarrow 0$ in $D > 1$ is unknown. For $h = 0$, it is a singlet (doublet) and belongs to the subspace $\sum_i^N S_i^z = 0$, N even ($\sum_i^N S_i^z = \frac{1}{2}$, N odd).¹⁶ For $h/J < (h/J)_c$ there is no gap between $|0\rangle$ and the continuum of excited states. At $(h/J) = (h/J)_c$ a gap Δ opens with $\Delta \sim [h/J - (h/J)_c]^s$, where in 1D $s = 1$ exactly.¹⁰ The value of $(h/J)_c$ is known exactly for all D to be¹⁷ $(h/J)_c = \frac{1}{2}z'$ where z' is the number of nearest neighbors. There is no order in 1D¹⁸; in 3D the order extends from some finite T_c down to $T = 0$.¹⁹ The case 2D is clearly a special one: for finite T the Mermin-Wagner theorem²⁰ excludes the existence of order. For $T = 0$ this theorem ceases to work and the existence of order is an open question. There exist also several estimates of the ground-state energy per spin ($h = 0$) of Eq. (2).²¹ Furthermore, it is known,¹ that for $h/J < (h/J)_c$ the Hamiltonian of Eq. (2) for $D > 1$ does not possess a simple $D + 1$ classical spin equivalence. The case $h = 0$ has been studied extensively in the past and was applied to a large number of experimental situations. An extensive list of references can be found in the article by Betts.²²

The Hamiltonian H [Eq. (2)] was already considered in Ref. 10 for the 1D case, where it has been found that the renormalization group (RG) method reproduces the exact solution²³ well. It is then natural to extend the study to higher dimensional cases where no exact solutions exist at present.

We shall address ourselves to the question of ordering, the structure of long-range correlation functions, calculation of critical ratios $(h/J)_c$, and rescaling properties of energy in 2D and partly in 3D. The calculations will be performed on different 2D lattices on the cubic lattice in 3D. The influence of shape and size of spin blocks used in the iterative procedure will be studied using 14 different spin blocks with up to $n_s = 27$ spins.

The paper is organized as follows. In Sec. II we

present the method as developed in Ref. 10 and specialized for 2D case. Similarities and differences with 1D case will be stressed. In Sec. III, we discuss the recursion relations for different blocks and lattices in $D = 2, 3$ and emphasize the existence of the special solutions (fixed cycles rather than fixed points). In Sec. IV the critical behavior of correlation functions for all values of h/J will be discussed. Sec. V is devoted to an approximative calculation of the ground-state energy. In Sec. VI we derive the recursion relations for the anisotropy γ and discuss the behavior of ordering as a function of γ in 2D. The general discussion and conclusions will be presented in Sec. VII. Finally, some analytic results which can be obtained for supercubic lattices for arbitrary D will be derived in Appendix A, while typical examples of recursion relations for the hexagonal lattice will be illustrated in Appendix B. The results on bipartite square and hexagonal lattices do not depend on the sign of J but the calculations on the triangular lattice will be here limited only to $J > 0$ case. In the case of $J < 0$ on the triangular lattice some kind of quantum frustration effect is expected²⁴ and this situation has been discussed elsewhere.²⁵

II. DESCRIPTION OF THE METHOD

In this section we adapt the formalism of Ref. 10 to the Hamiltonian Eq. (2) in $D > 1$. As usual we assume that at the iteration (n) the Hamiltonian can be written in the form

$$H^{(n)} = -\frac{1}{2}J^{(n)} \sum_{\langle ij \rangle} (S_i^{x(n)} S_j^{x(n)} + S_i^{y(n)} S_j^{y(n)}) - h^{(n)} \sum_i S_i^z + C^{(n)} \sum_i I_i^{(n)}, \quad (3)$$

where the initial values of $J^{(n)}$, $h^{(n)}$, and $C^{(n)}$ are

$$J^{(0)} = J, \quad h^{(0)} = h, \quad C^{(0)} = 0, \quad (4)$$

$I_i^{(n)}$ are unit matrices, $\langle ij \rangle$ represents a pair of nearest neighbors, and $C^{(n)}$ are constants. As in previous studies⁷⁻¹² we now group the spins into 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 neighboring blocks j, j' , $H_{jj'}^{(n)}$

$$H^{(n)} = \sum_j H_j^{(n)} + \sum_{\langle jj' \rangle} H_{jj'}^{(n)} + C^{(n)} \sum_j \sum_{p=1}^{n_s} I_{j,p}^{(n)}, \quad (5)$$

where

$$H_j^{(n)} = -\frac{1}{2}J^{(n)} \sum_{\langle pp' \rangle} (S_{j,p}^{x(n)} S_{j,p'}^{x(n)} + S_{j,p}^{y(n)} S_{j,p'}^{y(n)}) - h^{(n)} \sum_{p=1}^{n_s} S_{j,p}^z, \quad (6)$$

and

$$H_{j,j'}^{(n)} = -\frac{1}{2} J^{(n)} \sum_{\substack{p,p' \\ (j,p,j',p')}} (S_{j,p}^{x(n)} S_{j',p'}^{x(n)} + S_{j,p}^{y(n)} S_{j',p'}^{y(n)}) \quad (7)$$

In Eq. (7) j, j' is a pair of neighboring blocks, and the positions of spins within the blocks are denoted by p and p' . The first step in the renormalization-group (RG) procedure is to diagonalize exactly the spin-block Hamiltonian $H_j^{(n)}$. A number of lowest-lying states of a block is retained. They form a new, truncated basis in which the new parameters of the system are recalculated by pulling back the interblock couplings by $H_{j,j'}^{(n)}$. The whole procedure is iterated until under iteration no changes in the parameters are produced, i.e., until a fixed point of the RG transformation is reached. We shall limit ourselves in this study to keeping only two ($n_L \equiv 2$) lowest-lying states of a block, thereby ensuring that at each iteration the Hamiltonian takes the form of Eqs. (5)–(7). (As in Ref. 10, in $D > 1$ one could keep more levels, $n_L > 2$, at the cost of considerable calculational complications.) The search for the two lowest-lying states of $H_j^{(n)}$ with n_s spins is facilitated by observing that $[\Sigma_j^{(n)}, H_j^{(n)}] = 0$, where

$$\Sigma_j^{(n)} = \sum_{p=1}^{n_s} S_{j,p}^{z(n)} \quad (8)$$

and consequently the eigenstates of $H_j^{(n)}$ can be conveniently classified in terms of eigenvalues of $\Sigma_j^{(n)}$.

$H_j^{(n)}$ will be diagonalized in the basis of vectors of the form $|\epsilon_1, \dots, \epsilon_{n_s}\rangle$, where $\epsilon_p = \pm 1$ is the eigenstate of the z component of p th spin in the block. The matrix representation of $H_j^{(n)}$ in this basis will have a block-matrix form with n_s blocks. If we number the block matrices with q ($q = 1, \dots, n_s + 1$) then every block matrix is a representation of $H_j^{(n)}$ in the subspace ϵ_j^q corresponding to the eigenvalue

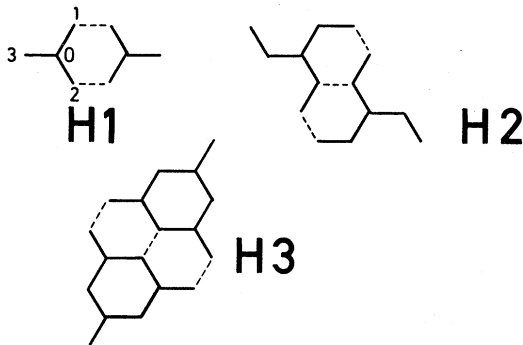


FIG. 1. Spin blocks and their couplings (dashed lines) on the hexagonal lattice.

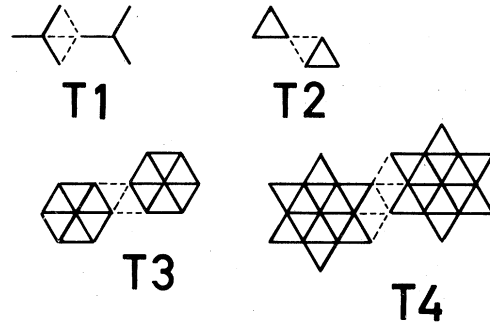


FIG. 2. Spin blocks and their couplings (dashed lines) on the triangular lattice.

$(-n_s + 2q - 2)$ of $\Sigma_j^{(n)}$. Let us denote by $|q\rangle$ the ground-state wave function of $H_j^{(n)}$ in the subspace ϵ_j^q . Since all the diagonal elements of $H_j^{(n)}$ in a given ϵ_j^q are equal to $(n_s - 2q + 2)h^{(n)}$, the ground-state energy E_q of $|q\rangle$ is equal to

$$E_q^{(n)} = (n_s - 2q + 2)h^{(n)} + e_q^{(n)} \quad (9)$$

$$q = 1, \dots, n_s + 1$$

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

$$-\frac{1}{2} \sum_{\langle p,p' \rangle} (S_{j,p}^{x(n)} S_{j,p'}^{x(n)} + S_{j,p}^{y(n)} S_{j,p'}^{y(n)})$$

For 2D blocks, which are not too large like $H1, T1, T2, Q1, Q2$ (see Figs. 1–3) all the e_q 's can be calculated by hand. For larger blocks only $e_1 = e_{n_s + 1}$ and

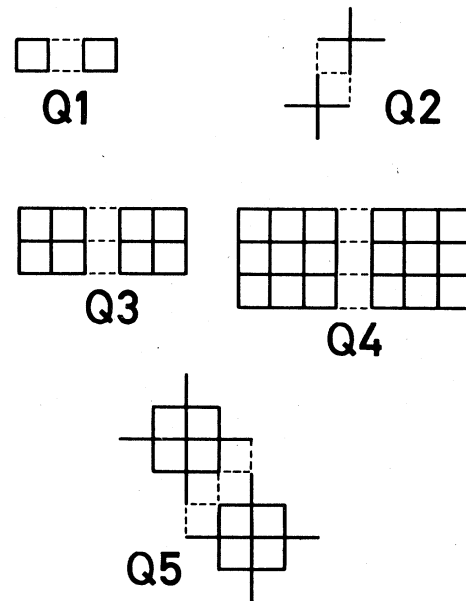


FIG. 3. Spin blocks and their couplings (dashed lines) on the square lattice.

$e_2 = e_{n_s}$ can be simply calculated. In fact, one can suitably generalize the 1D calculation and obtain the analytical expressions for $e_2 = e_{n_s}$ for a D -dimensional supercube with the edge length $l - 1$ ($n_s = l^D$) (see Appendix A). Certain other cases will be calculated by machine. As an illustration all the wave functions and associated energies E_q of a simple block $H1$ (see Fig. 1) with $n_s = 4$ spins will be derived in detail in Appendix B. The search for the two lowest-lying states of $H_j^{(n)}$ is simplified by noting that for a given $h^{(n)}/J^{(n)}$ they are always two lowest states of adjacent subspaces $\epsilon^q, \epsilon^{q+1}$. We introduce now the block spin operator \bar{S}_j by rewriting $H_j^{(n)}$ as

$$H_j^{(n)} = \frac{1}{2} (E_q^{(n+1)} - E_{q+1}^{(n+1)}) S_j^{z(n+1)} + \frac{1}{2} (E_q^{(n+1)} + E_{q+1}^{(n+1)}) I_j^{(n+1)} \quad (10)$$

$$\equiv -h^{(n+1)} S_j^{z(n+1)} + \frac{1}{2} (E_q^{(n+1)} + E_{q+1}^{(n+1)}) I_j^{(n+1)}, \quad (11)$$

where, using Eq. (9)

$$h^{(n+1)} = h^{(n)} + \frac{1}{2} (e_q - e_{q+1}) J^{(n)}. \quad (12)$$

In the above the states $|q\rangle$ and $|q+1\rangle$ are identified with "down" and "up" states of $S_j^{z(n+1)}$, called $|-\rangle^{(n+1)}$ and $|+\rangle^{(n+1)}$. The recursion relations for spin components are obtained by calculating the matrix elements of operators $\bar{S}_{j,p}^{(n)}$ between the block states $|\pm\rangle^{(n+1)}$. Depending on the position of spin in the block (p) we obtain, i.e., for the x component

$$S_{j,p}^{x(n)} = \xi_p^q S_j^{x(n+1)}, \quad (13)$$

and the same relation for y components.

The new coupling constant $J^{(n+1)}$ is obtained by computing the matrix elements of $H_{j,j'}^{(n)}$ between j and j' blocks. The form of the resulting sum depends on the shape of the blocks and will be separately determined in each case. For example, two blocks $Q3$ on the quadratic lattice (see Fig. 3) are linked with two bonds "corner-corner" and the one bond "face-face." Consequently

$$J^{(n+1)} = \xi_{qj} J^{(n)}, \quad (14)$$

with

$$\xi_{qj} = 2(\xi_{q,co})^2 + (\xi_{q,f})^2,$$

where

$$\xi_{q,co} = \langle + | S_{co}^{\alpha(n)} | - \rangle,$$

$$\xi_{q,f} = \langle + | S_f^{\alpha(n)} | - \rangle$$

($\alpha = X, Y$), and the subscripts co and f denoting a "corner" and "face" spin, respectively. The quantity ξ_{qj} does not depend on n . For a given subspace ϵ^q it

is then enough to compute a pair of recursion relations (12) and (14) which can be compactly written as

$$\left(\frac{h}{J} \right)^{(n+1)} = (\xi_{qj})^{-1} \left[\left(\frac{h}{J} \right)^{(n)} + \frac{1}{2} (e_q - e_{q+1}) \right]. \quad (15)$$

III. DISCUSSION OF RECURSION RELATIONS

The behavior of the recursion relations (15) is found by iterating them and finding the eventual limiting values, or fixed points, if any. The important observation to make now is that at every iteration step n one has to verify whether the resulting $(h/J)^{(n+1)}$ is still within the range of (h/J) for which the states $|q\rangle$ and $|q+1\rangle$ [used to derive $(h/J)^{(n+1)}$] are still the two lowest ones. The closer examination of spectra of all the blocks permits us to write down the conditions of validity of Eq. (15) for all the blocks of Figs. 1–4. Direct calculations indicate that for a given block and a given pair of neighboring subspaces, say ϵ^q and ϵ^{q+1} , the ground states E_q and E_{q+1} of these subspaces are the two lowest low-lying states of the set of *all* states belonging to ϵ^q and ϵ^{q+1} . The same statement can be made for any ϵ^q , in particular about ϵ^{q+1} and ϵ^{q+2} . The condition of validity of Eq. (15) can be obtained by equating $E_{q-1} = E_{q+1}$ for the lower limit and $E_q = E_{q+2}$ for the

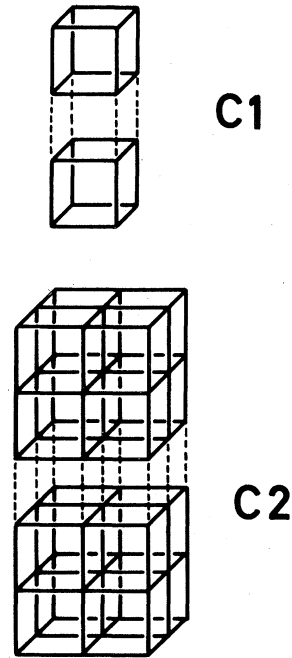


FIG. 4. Spin blocks and their couplings (dashed lines) on the cubic lattice.

higher limit. Using Eq. (9) one obtains

$$X_q < \left(\frac{h}{J}\right)^{(n)} < X_{q+1}, \quad (16)$$

where

$$X_q = \frac{1}{4}(e_{q+1} - e_{q-1}). \quad (17)$$

[For $q = n_s$ ($q = 1$) only the left (right) side of the inequality Eq. (16) remains.] The relation (16) tells us that we can proceed in iterating Eq. (15) as long as the values $(h/J)^{(n)}$ satisfy Eq. (16) for all n . There is an important difference between the 1D case¹⁰ and $D > 1$ cases considered here: in 1D for every q we can obtain a fixed point

$$\left(\frac{h}{J}\right)_q^* = \left(\frac{h}{J}\right)_q^{(n)} = \left(\frac{h}{J}\right)_q^{(n+1)}$$

whose value

$$\left(\frac{h}{J}\right)_q^* = \frac{e_{q+1} - e_q}{2(1 - \xi_{qj})} \quad (18)$$

satisfies Eq. (16), whereas in 2D and 3D the fixed points Eq. (18) for all q except $q = 1$ and $q = n_s$ lie always outside a corresponding region Eq. (16). Therefore the fixed points for $q \neq 1$, $q \neq n_s$ cannot be reached.

To compare 1D and 2D situations we present in Fig. 5 two sets of recursion relations for $h > 0$ for two blocks with $n_s = 9$: a chain of nine spins and the Q3 block on a quadratic lattice. [The structure of recursion relations as illustrated in Fig. 5(b) in 2D remains qualitatively the same for C1 and C2 blocks

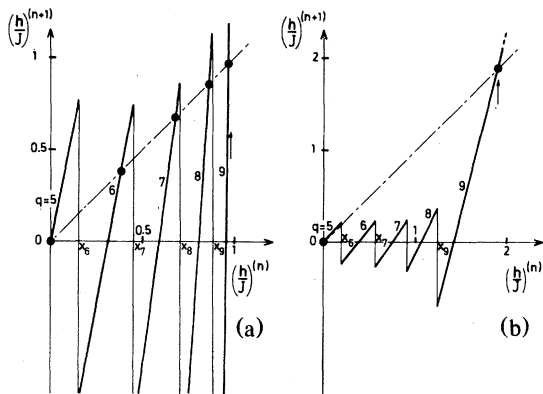


FIG. 5. Comparison of the $h > 0$ recursion obtained for two blocks of $n_s = 9$ spins: (a) a chain ($D = 1$) of nine spins, and (b) a $D = 2$ block Q3 (see Fig. 3). For (a) the fixed points (fat circles) are all unstable and are always inside the zones of validity or recursion relations, denoted by x_q , see Eqs. (16) and (17). For (b) only the last recursion relation cuts the bisecting line giving an unstable fixed point. The other relations do not give physical fixed points.

in 3D, see Fig. 4.] In 1D we have obtained in the range $|h/J| < 1$, $n_s = 9$ unstable fixed points, $(h/J)_q^*$. If the initial value was $(h/J)^{(0)} = (h/J)_q^*$ we always stay at this point with both $h^{(n)}$ and $J^{(n)}$ tending to zero. Since $h^{(\infty)} = 0$ the system has a gapless spectrum. If we chose $|(h/J)^{(0)}| > |(h/J)_K^*|$, with $K = 1$ or n_s , we find a gap Δ in the spectrum with $\Delta = 2h^{(\infty)}$ and $J^{(\infty)} = 0$, which corresponds to a stable fixed point characterizing a system of noninteracting spins in a field $h^{(\infty)}$. With $n_s \rightarrow \infty$ the unstable fixed points cover the segment $|h/J| < 1$ and coalesce into a line of fixed points. We can associate a set of critical exponents with every point of this line. They do not change along the line and undergo a jumplike change at $|h/J| = 1$, the exact value¹⁷ of the critical ratio. We stress that at every point of fixed line the exponents are well defined and their values are those of $(h/J) = 0$ point.

For $D = 2$ and 3, within the two-level scheme the situation is a bit different. Only the two last recursion relations $q = n_s$ and 1 can be iterated towards their fixed points $(h/J)_1^* = -(h/J)_{n_s}^*$. [These values correspond to the critical field $(h/J)_c = 1$ in 1D.] $(h/J)_c$ is known exactly¹⁷ in any D and is equal to

$$\left|\left(\frac{h}{J}\right)_c\right| = \frac{1}{2}z', \quad (19)$$

where z' is the number of nearest neighbors for a given lattice. [The formula (19) is to be modified for the antiferromagnetic interactions on a triangular lattice.²⁵] In Ref. 17 the formula (19) was derived by requiring that it be the highest magnetic field for which there is no gap between the ground state and continuum of excited states. In our RG calculations $(h/J)_{n_s}^*$ is an unstable fixed point above which the gap opens. Therefore $(h/J)_{n_s}^*$ can be associated with the critical field $(h/J)_c$.

No other recursion relations can be iterated towards their fixed points because they lie outside the range Eq. (17). From the more detailed numerical examination of a set of recursion relations, like Fig. 5(b) [with relation (17)] the following picture emerges: From whatever point $|(h/J)^{(0)}| < |(h/J)_c|$ one starts the iteration one is jumping between recursion relations with different q , not necessarily the neighboring ones. After a given number of iterations a small [with respect to $(h/J)_c$] region is reached in which only few recursion relations participate in the RG trajectory. By continuing the iterations the RG trajectory does not escape from this region. The size of this "fixed" region is roughly given by the position of zeros of the recursion relations lying closest to the origin; i.e., $h/J = 0$. The characteristic of this fixed region is slightly different for the blocks with n_s even or odd. For n_s even there are two recursion relations closest to the origin, numbered $q = \frac{1}{2}n_s$ and

$q = \frac{1}{2}n_s + 1$. If we start the iteration at any point within the limits of validity of either of them after a few iterations we end up in the small region $h/J \sim 0$. For certain ("commensurate") starting points, the fixed region consists of a close path where the same value of $(h/J)^{(n)}$ is reproduced every second n . For other ("incommensurate") starting points the fixed region is covered by the open, erratic RG trajectory. In Figs. 6(a) and 6(b), we present examples of the closed and erratic fixed trajectories as obtained using two central recursion relations of H1 block. Within this fixed region the values of $|(h/J)^{(n)}|$ never exceed 0.2. For n_s odd there exists always the recursion relation with $q_0 = \frac{1}{2}(n_s + 1)$ having (in most cases) an unstable fixed point $(h/J)_{q_0}^* = 0$. In this case three recursion relations q_0 and $q_0 \pm 1$ define a limited region around $h/J \approx 0$. Due to the presence of the central recursion relation in general no values $(h/J)^{(n)}$ reappear exactly in a course of iteration

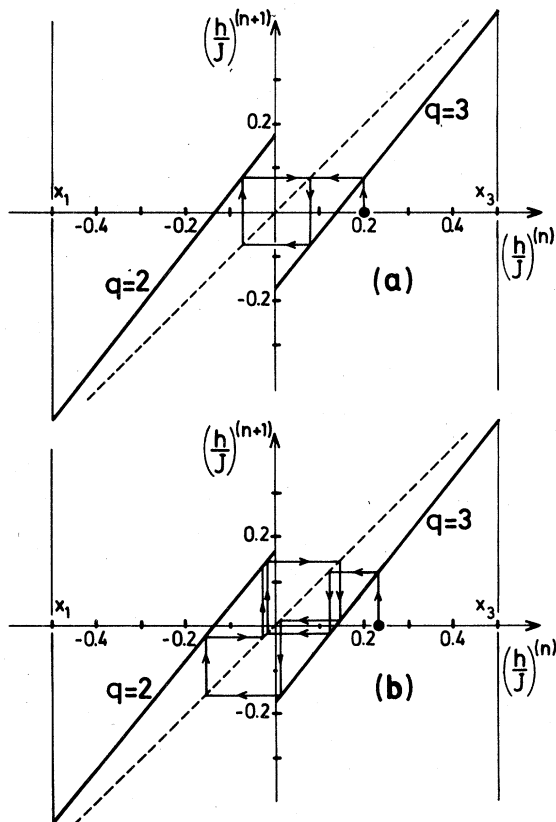


FIG. 6. Comparison of two RG trajectories for the $n_s = 4$, H1 block (see Fig. 1). The starting points of iterations are denoted by fat circles. Only a pair of recursion relations $q = 2, 3$ lying close to the origin are illustrated. The regions of validity are $x_2 = 0, x_1 = -x_3$. For (a) a closed trajectory is obtained enclosing a fixed region while for (b) an erratic RG trajectory encloses an "almost" fixed region.

although a fixed region can be defined with some spread $\delta((h/J)^{(n)}) \ll (h/J)_c$.

This last case is illustrated for the $n_s = 9$ (Q3 block of Fig. 3) in Fig. 7, where three recursion relations (obtained numerically) are represented, together with an example of an erratic RG trajectory. The distinction between n_s odd and n_s even cases becomes negligible by increasing n_s . With n_s increasing the fixed regions shrink progressively and in the limit $n_s \rightarrow \infty$ they coalesce to a stable fixed point $(h/J)^* = 0$. In a sense, the fixed region $(h/J) \cong 0$ is a finite-block-size effect. The above picture may be indicating that in the region $|h/J| < \frac{1}{2}z'$ the size of h/J is an irrelevant quantity and that the critical behavior of correlation functions in this region should be that of $h = 0$

We recall that, in a sense, a similar situation existed in 1D case,¹⁰ except that in the $|h/J| < 1$ region each point was a fixed point with exponents as of $h = 0$ situation. In 2D case no fixed points in $0 < |h/J| < \frac{1}{2}z'$ were found but the character of RG trajectories indicates that the exponents in this region were those of the $h = 0$ case. It is rather difficult at present to say whether the 2D results are resulting from the method or are the reflections of a deeper similarity between 1D and 2D situations. We tend to believe that the latter is true. Similar views were recently expressed, based on other methods.²⁶ On the other hand, the three-fixed-point structure of RG trajectory in 2D is strongly reminiscent of the Ising model in transverse field (IT).^{6,7} However one cannot draw any far reaching analogies between these two cases, particularly concerning the ordering. In 3D the calculations are limited by numerical possibilities. Only the block C1 was resolved completely and few recursion relations of C2 were obtained (see Fig.

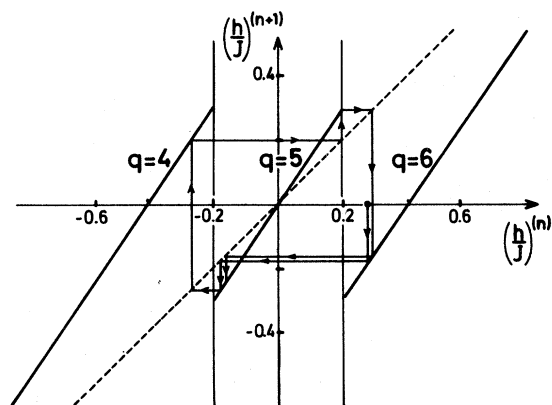


FIG. 7. An example of an erratic trajectory for three central recursion relations obtained numerically for the Q3 block (see Fig. 3). The starting point is depicted by a fat circle. The slope of the central relation was slightly increased for the reason of clarity.

4). In the $[(h/J)^{(n+1)}, (h/J)^{(n)}]$ plane the slopes of recursion relations are again smaller than in $D < 3$ cases. For $n_s \rightarrow \infty$ we may think of them as being piecewise approximants of continuous curves as in the IT model. Since in 3D the XY model orders,¹⁹ with the ordering extending to $T=0$ it could be instructive to analyze a block giving the fixed point $(h/J)^* = 0$. The smallest block with n_s odd leading to this fixed point is C2 with $n_s = 27$. Its subspace $\Sigma=0$ is too large to be diagonalized and the question of how the order in 3D could be treated was not pursued any more with our RG method.

IV. CRITICAL BEHAVIOR OF CORRELATION FUNCTIONS

In this section we will discuss in detail the results on different lattices and consequently the behavior of correlation functions will be calculated. For small enough blocks the magnetization $\mu_\alpha = \langle 0 | S_i^\alpha | 0 \rangle$ ($\alpha = X, Y$) can be directly computed using the spin recursion relations (13). The best way to avoid the edge effects is to evaluate the averaged magnetization $\bar{\mu}_\alpha$ of the block, with the corresponding operator $\sigma^\alpha = 1/n_s \sum_{p=1}^{n_s} S_p^\alpha$. Considering the q th recursion relation of Eq. (13) one obtains

$$\bar{\mu}_\alpha^{(n+1)} = \bar{\xi}_q \bar{\mu}_\alpha^{(n)}, \quad (20)$$

with

$$\bar{\xi}_q = \frac{1}{n_s} \sum_{p=1}^{n_s} \xi_{q,p}. \quad (21)$$

We find for $\alpha = X, Y$ and for all q 's of all the 2D blocks $\xi_q < 1$. It means that within our two-level ap-

proximations there is no magnetization for all the values of h in the 2D XY model. Further discussion on this point will be found in Sec. VII. For 3D blocks no recursion relations in the region $h/J \sim 0$ could be calculated but the slopes of other recursion relations seem to indicate a similarity with the Ising model with transverse field^{6,7} where the order exists. The results for $(h/J)_{n_s}^* = -(h/J)_1^* \equiv (h/J)_{\max}^*$ and the critical exponents as defined later, are presented in Table I for 2D and Table II for 3D.

Quantitatively the most satisfying results are obtained for the hexagonal lattice, with blocks $H1, H2, H3$. There is a monotonic approach of $(h/J)_{\max}^*$ towards 1.5 (exact value¹⁷). For the block $H3$ the deviation is $< 7.5\%$. We notice, that for $T2$ and $Q1$ we have obtained the exact position of the critical field. In these cases we have the exact cancellation of the error connected with the method and the error of introducing the blocks consisting of the surface only. For the quadratic lattice the blocks $Q1, Q3$, and $Q4$ represent the first three members of the sequence of hypersquares with the edge of length $l-1$ lattice spacings. A suitable generalization of the 1D case¹⁰ allows an analytic calculation of $(h/J)_{\max}^*$ and the exponents associated with it. The calculations are presented in Appendix A. For general D , we obtain from Eq. (A5)

$$\left(\frac{h}{J} \right)_{\max}^* = \frac{D \cos[\pi/(l+1)]}{1 - [2/(l+1)] \sin^2[\pi/(l+1)]} \xrightarrow{l \rightarrow \infty} 2. \quad (22)$$

We observe that for $l \rightarrow \infty$ we get for $(h/J)_{\max}^*$ the exact value 2. This means that concerning the values of $(h/J)_{\max}^*$ the method becomes exact in the limit of large hypercubes. The values of $(h/J)_{\max}^*$ gave us

TABLE I. The critical fields and critical exponents as obtained for the set of 2D blocks (Figs. 1, 2, and 3). \bar{z}_0 and $\bar{\eta}_{x0}$ denote the effective values averaged over a large number of iterations in the fixed regions near $h \approx 0$.

Block	$n_s = f^2$	$\frac{1}{2}z'$	$\left(\frac{h}{J} \right)_{\max}$	z_{\max}	z_0	\bar{z}_0	$\eta_{x\max}$	η_{x0}	$\bar{\eta}_{x0}$
H1	4	1.5	1.3	1.58	0.370	0.370	2.100	1.5150	1.5150
H2	7	1.5	1.333	1.4248			2.67		
H3	9	1.5	1.388	1.4649			2.082		
T1	4	3	3.16	0.6874			1.426		
T2	3	3	3.00	1.476	0.214	0.51	2.0	1.4762	1.76
T3	7	3	2.777	1.096	0.04534		2.042		
T4	13	3	2.6015	1.3800			2.1152		
Q1	4	2	2.0	1	0.4569	0.4569	2	1.4569	1.4569
Q2	5	2	1.6	1.2188	-0.1463	-0.1463	2.1309	1.3120	1.3120
Q3	9	2	1.8856	1.2618	0.144	0.191	2.0528	1.176	1.195
Q4	16	2	1.8774	1.4286			2.078		
Q5	13	2	1.636	1.9375			2.1381		

TABLE II. The critical fields and critical exponents as obtained for two 3D blocks (see Fig. 4) near $(h/J) \approx (h/J)_c$.

Block	$n_s = f^3$	$\frac{1}{2}z'$	$\left(\frac{h}{J}\right)_{\max}$	z_{\max}	$\eta_{x\max}$
C1	8	3	3	2	3
C2	27	3	2.828	2.523	3.182

much confidence for the method and we proceeded to calculate the correlation functions. Suppose now that we want to calculate the correlation function $\rho_{\vec{R}}^{\vec{x}} = \langle 0 | S_{\vec{0}}^{\vec{x}} S_{\vec{R}}^{\vec{x}} | 0 \rangle$ at the fixed point $(h/J)_q^*$ in D dimensions. For simplicity we assume that, in the units of lattice spacing, R is the n th power of the dilation factor $f = (n_s)^{1/D}$. Since there is no order we expect that at $(h/J)_q^*$, $\rho_{\vec{R}}^{\vec{x}}$ has a power-law behavior

$$\rho_{\vec{R}}^{\vec{x}} \xrightarrow{R \rightarrow \infty} R^{-\eta_{xq}^{(D)}}.$$

As in Eqs. (20) and (21) we introduce again the block-averaged quantity $\sigma_{\vec{R}}^{\vec{x}}$. Now

$$\rho_{\vec{R}}^{\vec{x}} \approx \langle 0 | \sigma_{\vec{0}}^{\vec{x}} \sigma_{\vec{R}}^{\vec{x}} | 0 \rangle$$

$$\eta_{\alpha\max}(D, l) = -D \ln \left[\frac{2}{l^2(l+1)} \left[\cotan \frac{\pi}{2(l+1)} \right]^2 \right] / \ln l \xrightarrow{l \rightarrow \infty} D, \quad (\alpha = X, Y), \quad (25)$$

$\eta_{\alpha\max}(D) = D$ is thus believed to be exact. We cannot, strictly speaking, repeat these calculations for any other values of $(h/J) < (h/J)_{\max}^*$, the reason being that no fixed points can be reached in this region. We can, however, quite formally calculate the corresponding quantity η_x without associating it with the correlation functions. The complexity of appropriate wave functions renders it practically impossible for larger blocks. For smaller blocks it can be done by hand. One observes that for all the recursion resulting η_x 's are smaller than D . In particular the recursion relation closest to origin (like for $H1$ block, see Fig. 6), or passing through origin (like for $T2$ block) gives values of η_x close to 1.5 in 2D. They are listed in Table I in the entry η_{x0} . No value of η_{x0} in 3D could be obtained. As explained in the previous section if we start the iteration at any point $(h/J) < (h/J)_{\max}^*$, after many steps we always end up at the fixed region about the origin, roughly given by the zeros of two recursion relations closest to the origin. In this region the RG trajectory jumps between these two recursion relations (n_s even, Fig. 6) or jumps between them and a one passing through origin (n_s odd, Fig. 7). It is then natural to associate with the fixed region a certain averaged exponent $\bar{\eta}_{x0}$

and we apply $n-1$ times the Eqs. (20) and (21). The new superspins $\bar{\sigma}_0^{(n)}$ and $\bar{\sigma}_R^{(n)}$ are now in the same block. The R dependence is obtained from

$$\begin{aligned} \langle 0 | \sigma_{\vec{0}}^{\vec{x}} \sigma_{\vec{R}}^{\vec{x}} | 0 \rangle &\approx (\bar{\xi}_q)^{2(n-1)} \xrightarrow{n \rightarrow \infty} (\bar{\xi}_q)^{2n} \\ &= R^{-\eta_{xq}^{(D)}} \end{aligned} \quad (23)$$

Now using the assumption that $R = n_s^{n/D}$ we get

$$\eta_{xq}(d) = -2D \frac{\ln \bar{\xi}_q}{\ln n_s} \quad (24)$$

The above formulas allow one to extract from the recursion relation q the exponent $\eta_{\alpha q}$ if the fixed point is reached. From the foregoing discussion only exponents near $(h/J)_c$ and near $(h/J) \approx 0$, referred to as $\eta_{\alpha\max}$ and $\eta_{\alpha 0}$, respectively, have a physical meaning. The calculated values of $\eta_{\alpha\max}$ are listed in Tables I ($D=2$) and II ($D=3$). We note that, except of $H3$ and $T1$ blocks, the values of $\eta_{x\max}$ are close to D . This is in full agreement with calculations based on the functional integral technique.^{27,28} The value $\eta_{x\max}(D) = \eta_x[(h/J)_c] = D$ is also obtained from the $l \rightarrow \infty$ limit of the D -dimensional supercube calculations with $n_s = l^D$ [see Eq. (A8)]:

which is simply an arithmetic average over a large number of interactions. If n_s is even we see from Table I that $\eta_{x0} = \bar{\eta}_{x0}$. For n_s odd $\bar{\eta}_{x0} > \eta_{x0}$, as in $Q3$, and $\bar{\eta}_{x0}$ seems to be not far from $\frac{3}{2}$. This value of $\bar{\eta}_{x0}$ is best reproduced by the simple block $H2$ which is also known to give the best results in other RG calculations.⁷

The method allows also an independent evaluation of the dynamical critical exponent z which, at the fixed point, is defined as $H^{(n+1)} = f^{-z} H^{(n)}$ or

$$J^{(n+1)} = f^{-z} J^{(n)}, \quad (26)$$

where $f = n_s^{1/D}$ is a dilation factor and $J^{(n+1)}$ is defined in Eq. (14). At the fixed point the $h^{(n)}$'s and the $J^{(n)}$'s rescale with the same factor so it is enough to use for instance Eq. (14) to obtain z at the fixed point $(h/J)_q^*$ as

$$z_q = -D \frac{\ln \xi_{qJ}}{\ln n_s} \quad (27)$$

Again we have to distinguish between the fixed point $(h/J)_{\max}^*$ and fixed regions around $h/J \sim 0$. The values of z_{\max} , z_0 , and \bar{z}_0 are listed in Table I. To date, no calculations of z_0 for $D > 1$ were reported so

our values $z_0 \sim \frac{1}{3}$ in 2D are the first estimates of z_0 . In contrast to z_0 , z_{\max} was estimated to be equal 2 for all $D > 1$.^{27,28} Our results are based on a two-level method which does not describe the energetic well. The error can be best estimated by performing the $l \rightarrow \infty$ limit of Eq. (A6) for the supercubes. One obtains

$$z_{\max} = -\ln \left[\frac{2}{l+1} \left(\sin \frac{\pi}{l+1} \right)^2 \right] \Bigg|_{l \rightarrow \infty} \rightarrow 3, \quad (28)$$

which does not agree with estimates of Gerber and Beck.²⁷ By taking more levels at each iteration the results will be surely improved as was already shown in the 1D case.¹⁰

V. ESTIMATES OF THE GROUND-STATE ENERGY

In this section we shall present a calculation of ground-state energy estimates. For n_s unpair and $h \rightarrow 0$, there is a fixed point $(h/J)_{q_0}^* = 0$ with $q_0 = \frac{1}{2}(n_s + 1)$, $\xi_{q_0 J} \equiv \xi_J$, and $e_{q_0} = e_{q_0+1} \equiv e_0$. At every stage iteration n we use the energies per number of spins, i.e., n_s^n . The geometrical series is readily summed to give [see Eqs. (5), (9), and (11)]

$$\left[\frac{E_0(h=0)}{JN} \right]_S = \frac{e_0}{n_s - \xi_J}. \quad (29)$$

$$\frac{E_0}{N} = \frac{1}{2} z' \lim_{n \rightarrow \infty} \sum_{n=0}^n \frac{(n_s - 2q + 1)h^{(n)} + \frac{1}{2}(e_q + e_{q+1})J^{(n)}}{b(n+1)}. \quad (30)$$

Equation (30) is a generalization of Eq. (20) of Ref. 10 for $D > 1$ cases. In order to sum Eq. (30) the explicit form of $b(n)$ must be known. It can be shown by induction that for every lattice and block we considered the $b(n)$'s satisfy the following recursion relation

$$b(n+1) = n_s b(n) + B_0 \bar{l}^n, \quad b(0) \equiv 0, \quad (32)$$

where n_s is a number of spins at stage 1, B_0 is a number of bonds in the block at stage 1, and \bar{l} is the number of

TABLE III. The values of $h=0$ estimates of the ground-state energies per spin together with quantities used to derive it, see Eq. (33). $-\bar{E}_0/N$ is an average $-(E_{0B} + E_{0S})/2N$. In the last column several existing estimates for $-E_0/N$ are quoted.

Block	$\frac{1}{2}z$	(n_s, \bar{l}, B_0)	ξ_J	$-e_0$	$\left[-\frac{E_0}{N} \right]_B$	$\left[-\frac{E_0}{N} \right]_S$	$-\frac{\bar{E}_0}{N}$	$-\left[\frac{E_0}{N} \right]_{\text{est}}$
Q2	2	(5,3,4)	1.125	2.449	1.436	0.630	1.033	$\left\{ \begin{array}{l} 1.098^a \\ 1.08^b \\ 1.074^c \end{array} \right.$
Q3	2	(9,3,12)	0.853	7.187	1.291	0.882	1.087	
T2	3	(3,2,3)	0.889	2.00	2.469	0.947	1.708	1.58 ^d
T3	3	(7,3,12)	0.957	6.760	1.874	1.119	1.496	

^aReference 21.

^bReference 35.

The values calculated from Eq. (28) are not satisfactory (see Table III). While this simple device works in 1D, it cannot give good results in 2D for the following reasons: First, we observe that the identity relating the number of bonds with number of spins in an infinite system, $N_B = \frac{1}{2}z'N_s$, is no longer satisfied for a superblock at stage n , when for $n < \infty$ $N_B^{(n)} > \frac{1}{2}z'N_s^{(n)}$. To account for this bond-site asymmetry we have chosen to calculate at every stage the ground state energy *per bond* and to sum all the contributions. The energy per spin is given by the resulting sum multiplied by $\frac{1}{2}z'$. If the number of bonds at stage n is $b(n)$ [with $b(0) = 0$] then from Eqs. (9) and (11) the constants $C^{(n)}$ of Eq. (5) satisfy

$$\frac{C^{(n+1)}}{b(n+1)} = \frac{C^{(n)}}{b(n)} - \frac{(n_s - 2q + 1)h^{(n)} + \frac{1}{2}(e_q + e_{q+1})J^{(n)}}{b(n+1)}. \quad (30)$$

The total ground-state energy per bond E_0/N_B is the sum of Eq. (30), and consequently the energy per spin is

^cReference 34.

^dReference 37.

bonds between two neighboring blocks at stage 1. For example, for the $T3$ block $(n_s, B_0, \bar{l}) = (7, 12, 3)$. We seek the solution in the form $b(n) = xn_s^n + y\bar{l}^n$ and we find

$$b(n) = \frac{B_0}{n_s - \bar{l}} (n_s^n - \bar{l}^n), \quad (33)$$

which can be used to calculate $E_0(h)/N$ for arbitrary h . Only the case $h=0$ on the blocks with n_s odd: $Q2$, $Q3$, and $T2$ will be calculated. For n_s unpair, using Eqs. (31) and (33) we get

$$\left(\frac{E_0(h=0)}{JN} \right)_B = e_0 \frac{n_s - \bar{l}}{B_0} \frac{1}{2} z' \lim_{n \rightarrow \infty} \left(\sum_{n=0}^n \frac{(\xi_j)^n}{n_s^{n+1} - \bar{l}^{n+1}} \right). \quad (34)$$

The values calculated with Eq. (34) are given in Table III.

Evidently, these values are not variational in character because the bond-site asymmetry can be remedied in other ways. Since the derivation of Eq. (29) [Eq. (34)] underestimates (overestimates) the role of bonds we have simply taken the arithmetic average of Eqs. (29) and (34). The results are presented in Table III and it is seen that indeed a very good agreement with existing estimates was achieved.

VI. ANISOTROPY DEPENDENCE OF MAGNETIZATION

In this section the numerical results concerning the vanishing of order as a function of anisotropy will be presented. To this end we set in Eq. (1) $J \equiv 1$ and $h=0$ and rewrite Eq. (1) at stage n of iteration as

$$H^{(n)} = - \left[\sum_{\langle ij \rangle} \frac{1}{2} (1 + \gamma^{(n)}) S_i^{x(n)} S_j^{x(n)} + \frac{1}{2} (1 - \gamma^{(n)}) S_i^{y(n)} S_j^{y(n)} \right]. \quad (35)$$

where

$$K^{(n+1)}(\gamma^{(n)}) = \frac{1}{2} (1 + \gamma^{(n)}) [\xi^x(\gamma^{(n)})]^2 + \frac{1}{2} (1 - \gamma^{(n)}) [\xi^y(\gamma^{(n)})]^2, \quad (40a)$$

and

$$\gamma^{(n+1)}(\gamma^{(n)}) = \left\{ \frac{1}{2} (1 + \gamma^{(n)}) [\xi^x(\gamma^{(n)})]^2 - \frac{1}{2} (1 - \gamma^{(n)}) [\xi^y(\gamma^{(n)})]^2 \right\} / K^{(n+1)} \quad (40b)$$

The levels $|\pm\rangle$ and the relations (40) were determined numerically for the blocks $T3$ and $Q3$ in order to calculate $\mu^x = \mu^x(\gamma)$ in the limit $\gamma \rightarrow 0$. It was found that

$$\mu^x \underset{\gamma \rightarrow 0}{\sim} \gamma^{0.20}$$

We choose the representation of eigenfunctions of S^x . Similarly to IT case^{6,7} the spectrum of Eq. (35) can be decomposed into two subspaces with opposite parity total number of "down" spins. For a given block we denote the ground states of these subspaces $|+\rangle$ and $|-\rangle$, respectively. The wave functions $|\pm\rangle$ can be developed in the basis of vectors in the form $|\epsilon_1, \epsilon_2, \dots, \epsilon_{n_s}\rangle$, where $\epsilon_K = \pm 1$ for $S_K^{x(n)} = \pm 1$

$$|\pm\rangle^{(n+1)} = \sum^{\pm} \lambda_{\epsilon_1, \dots, \epsilon_{n_s}}^{\pm(n)} |\epsilon_1, \dots, \epsilon_{n_s}\rangle, \quad (36)$$

where \sum^{\pm} denotes the summations restricted to above two subspaces. For n_s odd the spectrum consists of series of doublets, $|+\rangle$ and $|-\rangle$ being the lowest lying pair of them; also, it turns out that $\lambda^+ = \lambda^-$. The recursion relation defining block spins are obtained by calculating for peripheral spins $S_p^{\alpha(n)}$ ($\alpha = x, y$) their matrix elements

$$\langle - | S_p^{\alpha(n)} | + \rangle = \xi_p^{\alpha(n)} (\{\lambda_i^{\pm}\}) .$$

New couplings $\gamma^{(n+1)}$ are obtained by rewriting

$$H^{(n+1)} = - \frac{1}{2} [1 + \gamma^{(n)} (\xi^x)^2] \sum_{\langle ij \rangle} S_i^{x(n+1)} S_j^{x(n+1)} - \frac{1}{2} [1 - \gamma^{(n)} (\xi^y)^2] \sum_{\langle ij \rangle} S_i^{y(n+1)} S_j^{y(n+1)}, \quad (37)$$

with

$$(\xi^{\alpha(n)})^2 \equiv \sum_{\substack{p \in i \\ p' \in j \\ (p, p')}} \xi_p^{\alpha(n)} \xi_{p'}^{\alpha(n)}, \quad \alpha = x, y, \quad (38)$$

where in Eq. (38) the summation is over the peripheries of neighboring blocks i, j . (For the sake of simplicity we do not consider the more complicated cases, like block $T1$, see Fig. 2.)

Equation (37) can be now rewritten as

$$H^{(n+1)} = -K^{(n+1)} \sum_{\langle ij \rangle} \left[\frac{1}{2} (1 + \gamma^{(n+1)}) S_i^{x(n+1)} S_j^{x(n+1)} + \frac{1}{2} (1 - \gamma^{(n+1)}) S_i^{y(n+1)} S_j^{y(n+1)} \right], \quad (39)$$

for $Q3$ and

$$\mu^x \underset{\gamma \rightarrow 0}{\sim} \gamma^{0.22}$$

for $T3$. This is consistent with the results in Sec. IV where also no order was found within the two-level method in the isotropic case. It is not clear to what extent the $\mu^x(\gamma)$ dependence can be trusted because we used degenerate levels in the RG procedure. In 1D it was found exactly^{23, 29, 30} that

$$\mu^x(\gamma) \underset{\gamma \rightarrow 0}{\sim} \gamma^{1/4}$$

VII. DISCUSSION AND CONCLUSIONS

As mentioned in the Introduction the 2D XY model at $T=0$ presents a very special case: for $h=0$, Eq. (2), there may exist a phase transition in the ground state as function of spin dimensionality s , because for $s = \frac{1}{2}$ the order may not exist but it certainly exists for $s = \infty$. Furthermore, for fixed $s = \frac{1}{2}$ there must exist a phase transition in the ground state for $1 < D < 3$, since $D=1$ case is not ordered, whereas $D=3$ case is.¹⁹ (Let us mention that the analysis at $T \neq 0$ situations are also plagued with similar difficulties.³¹⁻³³)

We have applied the two-level renormalization group for all the values of (h/J) . We hope to have shown that the method becomes asymptotically exact at $(h/J)_c$ as far as the behavior of correlation functions is concerned in the limit of infinitely large hypercubic blocks. The analytical calculations for the hypercubes of Appendix A can be extended to other types of lattices²⁵ with the same results. At the $(h/J)_c$ the gap opens with the exponents $s=1$. We believe that $s=1$ in all D exactly. From the exact scaling law at $(h/J)_c = \frac{1}{2}z'$, $s = z\nu$ and presumed equality $z=2$ (all D)²⁷ we obtain the divergence of the correlation length $R_c \sim [h/J - (h/J)_c]^{-\nu}$ with $\nu = D^{-1}$. The power-law behavior of $\rho_x(R)$ is described by $\eta = D$ at $(h/J)_c$. The above values of $(h/J)_c$ and η_{\max} are reasonably well reproduced in $D=2$ and 3 . In the region $|h/J| < |(h/J)_c|$, contrary to the 1D case,¹⁰ no fixed points were obtained and for $n_s \rightarrow \infty$ the system is mapped into the $h=0$ case. We have no reasons to believe that the method is exact for $h=0$. In fact the $h=0$ results are, in a sense, obtained as an extrapolation from the $h \neq 0$ situation. There are many indications that for $h=0$ the ground-state wave function $|0\rangle$ is extremely complicated. Recently, a considerable effort was undertaken to reconstruct $|0\rangle$. The variational approach³⁴ and the extrapolation from the finite cell data³⁵ both lead to some degree of order in $|0\rangle$. It is not clear at the moment whether it is a result of approximations used or a reflection at ordering in the true ground

state. Our method in its present form did not detect any ordering which is surely a very subtle effect. In contrast, the values of ground-state energy (corrected for surplus of bonds in blocks) are not in disagreement with existing estimates. Since no order was observed we assumed for $h=0$ as a hypothesis a power-law behavior of spin-spin correlation functions. The corresponding exponents η_0 were calculated in $D=2$ for several blocks and their values lie roughly in the interval $1.2 \leq \eta_0 \leq 1.6$. The corresponding dynamic exponents z_0 are calculated to be $0.2 < z_0 < 0.45$ depending on the block.

Let us emphasize that the numbers quoted above are tentative. They are merely the best we have been able to achieve with the two-level renormalization-group procedure.

We have already noticed that there exists a certain similarity between the $h \neq 0$ behavior in $D=1$ and 2 : in $D=1$ the exponents $(\eta_{x_0, z_0}) = (\frac{1}{2}, 1)$ were constants all the way along the line of fixed points $0 < |h/J| < 1$. In $D=2$ the RG recursion relations map any point $0 < |h/J| < \frac{1}{2}z'$ into the stable fixed point $(h/J)^* = 0 (n_s \rightarrow \infty)$, with the exponents $(\eta_{x_0, z_0}) \approx (\frac{3}{2}, \frac{1}{3})$. It is then reasonable to assume that for $D=1, 2$ and $h=0$ the space-time correlation functions can be written in a scaled form:

$$\begin{aligned} \rho_B^g(R, t) &= \langle 0 | S_B^g(0) S_B^g(t) | 0 \rangle \\ &= R^{-\eta_D} F_D \left[\frac{t^D}{R} \right] \quad (\alpha = x, y), \end{aligned} \quad (41)$$

where $F_D(X)$ is the scaling function in D dimensions and the subscripts "0" have been suppressed. Equation (41) may also serve as the definition of (η_D, z_D) . F_D is assumed to be nonsingular.

It is now very interesting to show that both pairs of (η_D, z_D) , $D=1, 2$ follow directly from the explicit form of $\rho_D(R, t)$ derived very recently by Luther²⁶:

$$\rho_B^g(R, t) \sim [R^{D-1}(R^2 - t^2)^{1/4}]^{-1} \quad (D=1, 2) \quad (42)$$

Equation (42) was worked out by generalization to $D=2$ of the bosonization procedure of Luther and Peschel.³⁶ In order to associate Eq. (42) with the form Eq. (41) we have to assume that

$$F_D(X) \underset{X \rightarrow 0}{\rightarrow} \text{const}$$

We then obtain from Eq. (42) $\eta_D = D - \frac{1}{2}$, ($D=1, 2$), in agreement with our estimates. To get the z_0 's we observe that for $R \rightarrow 0$ ρ_D should depend on t only. Then, it is necessary that

$$F_D(X) \underset{X \rightarrow \infty}{\rightarrow} X^{-\eta_D},$$

or

$$\rho_D(t) \underset{t \rightarrow \infty}{\rightarrow} t^{-z_D \eta_D},$$

with Eq. (41) giving $z_D \eta_D = \frac{1}{2}$. Substituting the previous values of η_D we obtain $z_1 = 1$, $z_2 = \frac{1}{3}$, again in fair agreement with our results. While the above cannot serve as a proof of Eq. (42) we do think that the agreement between two such different approaches as RG and the bosonization is an encouraging sign. Clearly the region $h \sim 0$ must still be treated with more refined methods in order to test the above results. It is entirely possible that the treatment of ordering in the 2D XY model would require a more powerful method which is not known at present.

ACKNOWLEDGMENTS

One of us (K.A.P.) thanks Professor J. Friedel for help and encouragement and thanks the Deutsche Forschungsgemeinschaft, Bonn for a research fellowship. We thank Professor A. Luther for permission in quoting his unpublished results and we thank him and Professor B. Simon for useful discussions.

APPENDIX A: ANALYTICAL EXPRESSIONS FOR THE CRITICAL FIELD LOCATION AND THE EXPONENTS AT THE CRITICAL FIELD FOR THE HYPERCUBIC LATTICE IN D DIMENSIONS

Here, we applied the method by considering hypercubic blocks with l spins in each direction. The total number of spins in the block is $n_s = l^D$ and a given spin in the block can be labeled by the D numbers p_1, \dots, p_D where $p_i = 1, \dots, l$. To find the location of the critical field we construct the RG transformation which considers the states $|+\rangle$ and $|-\rangle$, respectively, ground states of the subspaces $q = n_s + 1$ and $q = n_s$. The state $|+\rangle$ is unique and corresponds to all the z -spin components pointing up. The state $|-\rangle$ is a given combination of the elementary functions Φ_{p_1, \dots, p_D} which correspond to all the spins pointing up except the spin located in p_1, \dots, p_D pointing down. The right normalized combination which corresponds to the ground state of the XY Hamiltonian at step n (in the subspace $q = n_s$) is:

$$|-\rangle = \sum_{p_1, \dots, p_D} \left(\frac{2}{l+1} \right)^{D/2} \times \sin \frac{p_1 \pi}{l+1} \cdots \sin \frac{p_D \pi}{l+1} \Phi_{p_1, \dots, p_D} \quad (\text{A1})$$

The reduced energies e_{n_s+1} and e_{n_s} [Eq. (9)] are

$$e_{n_s+1} = 0, \quad e_{n_s} = -eD \cos \frac{\pi}{l+1}, \quad (\text{A2})$$

respectively. Also by expressing the old spin operators we find that

$$S_{p_1, \dots, p_D}^x = \xi_{p_1, \dots, p_D} S^{x(n+1)},$$

with

$$\xi_{p_1, \dots, p_D} = \left(\frac{2}{l+1} \right)^{D/2} \sin \frac{p_1 \pi}{l+1} \cdots \sin \frac{p_D \pi}{l+1} \quad (\text{A3})$$

The renormalization of the constant J is obtained by rewriting the interblock interaction which involves all the spins of one face of the hyperblock. We get:

$$\begin{aligned} \xi_J &= \frac{J^{(n+1)}}{J^{(n)}} = \sum_{p_2, \dots, p_D} \xi_{1, p_2, \dots, p_D}^2 \\ &= \frac{2}{l+1} \left[\sin \frac{\pi}{l+1} \right]^2. \end{aligned} \quad (\text{A4})$$

The location of the last fixed point is then given by:

$$\left(\frac{h}{J} \right)_{\max}^* = D \cos \frac{\pi}{l+1} \left[1 - \frac{2}{l+1} \left[\sin \frac{\pi}{l+1} \right]^2 \right], \quad (\text{A5})$$

The exponent z at the fixed point is given by:

$$z = -\ln \left[\frac{2}{l+1} \left[\sin \frac{\pi}{l+1} \right]^2 \right] / \ln l. \quad (\text{A6})$$

One can also find the exponent η by evaluating $\bar{\xi}$ [Eq. (21)]

$$\begin{aligned} \bar{\xi}_{n_s} &= \frac{1}{l^D} \sum_{p_1, \dots, p_D} \left(\frac{2}{l+1} \right)^{D/2} \\ &\quad \times \sin \frac{p_1 \pi}{l+1} \cdots \sin \frac{p_D \pi}{l+1}, \end{aligned} \quad (\text{A7})$$

we find:

$$\eta_{\alpha \max} = -D \ln \left[\frac{2}{l^2(l+1)} \left[\cotan \frac{\pi}{2(l+1)} \right]^2 \right] / \ln l. \quad (\text{A8})$$

When $l \rightarrow \infty$ we find:

$$\begin{aligned} \left(\frac{h}{J} \right)_{\max}^* &\rightarrow D = \frac{1}{2} z', \quad \left(\frac{h}{J} \right)_{\max}^* \rightarrow \left(\frac{h}{J} \right)_c, \\ z &\rightarrow 3, \\ \eta &\rightarrow D. \end{aligned} \quad (\text{A9})$$

The results for $(h/J)_c$ and η are asymptotically exact. The result for z is wrong; we think that z must tend to 2. To have a good estimation of z we must take more levels.

APPENDIX B: DERIVATION OR RECURSION
RELATIONS FOR THE BLOCK H_1

The block H_1 has $n_s = 4$ spins and is coupled with its neighboring block by two peripheric-peripheric couplings, as illustrated in Fig. 1. According to Eq. (9) the ground-state energies E_q of five different subspaces of the single block Hamiltonian,

$$H_{H_1} = -J[S_0^+(S_1^- + S_2^- + S_3^-) + S_0^-(S_1^+ + S_2^+ + S_3^+)] - h(S_0^z + S_1^z + S_2^z + S_3^z) \quad (\text{B1})$$

satisfy at the n th iteration

$$E_q^{(n)} = (6 - 2q)h^{(n)} + e_q J^{(n)}, \quad (\text{B2})$$

$$q = 1, \dots, 5.$$

As usually, the noramalized wave functions $|q\rangle$ corresponding to E_q 's will be chosen using the criterium that for a given q they must have the *highest possible symmetry of the block*. We use the representation of eigenfunctions of $\Sigma^z = \sum_{k=0}^3 S_k^z$. Below we give the set of $|q\rangle$'s and E_q 's of H_1 :

$$q = 1: |1\rangle = \begin{pmatrix} - \\ - \\ - \\ - \end{pmatrix} \equiv \psi_1, \quad E_1 = 4h + 0J, \quad e_1 = 0,$$

$$q = 2: |2\rangle = \frac{1}{\sqrt{2}} \left\{ \begin{pmatrix} - \\ + \\ - \\ - \end{pmatrix} + \frac{1}{\sqrt{3}} \left[\begin{pmatrix} + \\ - \\ - \\ - \end{pmatrix} + \begin{pmatrix} - \\ - \\ - \\ + \end{pmatrix} + \begin{pmatrix} - \\ - \\ + \\ - \end{pmatrix} \right] \right\} \equiv \frac{1}{\sqrt{2}} (\psi_2 + \psi_3),$$

$$E_2 = 2h - \sqrt{3}J, \quad e_2 = -\sqrt{3},$$

$$q = 3: |3\rangle = \frac{1}{\sqrt{6}} \left[\begin{pmatrix} - \\ + \\ + \\ + \end{pmatrix} + \begin{pmatrix} + \\ + \\ - \\ - \end{pmatrix} + \begin{pmatrix} + \\ - \\ + \\ - \end{pmatrix} + \begin{pmatrix} - \\ + \\ - \\ - \end{pmatrix} + \begin{pmatrix} + \\ + \\ - \\ - \end{pmatrix} + \begin{pmatrix} - \\ + \\ - \\ + \end{pmatrix} \right] \equiv \psi_4, \quad (\text{B3})$$

$$E_3 = 0h - 2J, \quad e_3 = -2,$$

$$q = 4: |4\rangle = \frac{1}{\sqrt{2}} \left\{ \begin{pmatrix} + \\ - \\ + \\ + \end{pmatrix} + \frac{1}{\sqrt{3}} \left[\begin{pmatrix} - \\ + \\ + \\ + \end{pmatrix} + \begin{pmatrix} + \\ + \\ + \\ - \end{pmatrix} + \begin{pmatrix} + \\ + \\ - \\ + \end{pmatrix} \right] \right\} \equiv \frac{1}{\sqrt{2}} (\psi_5 + \psi_6),$$

$$q = 5: |5\rangle = \begin{pmatrix} + \\ + \\ + \\ + \end{pmatrix} \equiv \psi_7, \quad E_5 = -4h - 0J, \quad e_5 = 0.$$

In the truncated basis $\psi_1 \cdots \psi_7$ H_{H_1} has the following matrix representation

ψ_1	ψ_2	ψ_3	ψ_4	ψ_5	ψ_6	ψ_7	
ψ_1	$-4h$						$q = 5, \Sigma^z = +4$
ψ_2	$-2h$	$-\sqrt{3}J$					$q = 4, \Sigma^z = 2$
ψ_3	$-\sqrt{3}J$	$-2h$					
ψ_4			$-2J$				$q = 3, \Sigma^z = 0$
ψ_5				$2h$	$-\sqrt{3}J$		$q = 2, \Sigma^z = -2$
ψ_6				$-\sqrt{3}J$	$2h$		$q = 1, \Sigma^z = -4$
ψ_7						$4h$	

(B4)

from which the above values of E_q follow. We note that the search of the ground state reduces to solving a 2×2 matrix. The remaining nine orthonormal functions $\psi_8 \dots \psi_{16}$ completing the full basis of H_{H1} are completely decoupled from $\psi_1 \dots \psi_7$ and describe higher excited states.

The recursion relations between $q = 4$ and 5 subspaces are obtained from Eqs. (B3):

$$h^{(n+1)} = h^{(n)} + \frac{1}{2}(e_4 - e_5)J^{(n)} = h^{(n)} - \frac{1}{2}\sqrt{3}J^{(n)},$$

$$J^{(n+1)} = \frac{1}{3}J^{(n)}. \quad (\text{B5})$$

The fixed point resulting from Eq. (B5) is $(h/J)_4^* = 1.299$ and lies in the region of validity of Eq. (B5) from Eq. (17) by $(h/J)_4^* > \frac{1}{4}(e_5 - e_3)$, so $(h/J)_4^* > \frac{1}{2}$ and $(h/J)_4^*$ can therefore be regarded as a "physical" fixed point with the critical exponents $\eta_{x4} \equiv \eta_{x\max} = 2.1$ and $z_4 \equiv z_{\max} = 1.58$. In contrast, the fixed point of recursion relations between $q = 3$ and 4 subspaces, $(h/J)_3^*$, as obtained from

$$h^{(n+1)} = h^{(n)} + \frac{1}{2}(e_3 - e_4) = h^{(n)} - 0.134J^{(n)},$$

$$J^{(n+1)} = \frac{7 + 2\sqrt{12}}{18}J^{(n)}, \quad (\text{B6})$$

is $(h/J)_3^* = 0.5917$ and does *not* satisfy $0 < (h/J)_3^* < \frac{1}{2}$. This implies that $(h/J)_3^*$ cannot be regarded as a "physical" fixed point. One can, however, attach some meaning to the exponents. In fact, if we start the iteration at any point $|h/J| < \frac{1}{2}$ after a number of steps we end up in a "fixed" region between (3,4) and (2,3) recursion relations, roughly limited by $|h/J| < 0.075$. This situation is illustrated in Fig. 6. As explained above it is then reasonable to introduce "averaged" exponents which are arithmetic averages over the number of iterations. In this particular example the "averaged" exponents are equal to those related to *either* of (3,4) and (2,3) recursion relations. The above example on the hexagonal lattice is certainly a very simple one. The determination of wave functions $|q\rangle$ for larger blocks becomes quickly unmanageable and exceeds even numerical possibilities for $n_s > 9$ in 2D and $n_s > 8$ in 3D [for the $Q5(n_s = 13)$ block the evaluation of (6,7) recursion relations would require the diagonalization of 1716-dimensional matrix]. It is very advantageous, however, that the evaluation of $(h/J)_{n_s}^* = (h/J)_{\max}^*$ is made by hand for *all the blocks* listed in Tables I and II.

*Laboratoire associé au CNRS.

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