Real-space renormalization group and critical phenomena in the two-dimensional spin-$\frac{1}{2}$ X-Y model

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A new formulation of the renormalization-group in real space, suitable for quantum spin systems is proposed. The method is applied to the two-dimensional spin-$\frac{1}{2}$ X-Y model on a triangular lattice, the renormalization-group transformation being evaluated up to second order in an appropriate cumulant expansion. To first order an unstable fixed point of the transformation is found, corresponding to a critical temperature and critical indices in satisfactory qualitative agreement with present high-temperature series expansion estimates. In the second-order calculation, however, this fixed point disappears, thus throwing some doubt on the conventional picture of criticality as furnished by high-temperature series. The free energy of the model is also computed. For relatively small values of the nearest-neighbor coupling it is in good agreement with that found by high-temperature series analysis.

In recent years considerable efforts have been made to obtain definite evidence for a phase transition in two-dimentional X-Y and Heisenberg spin models.

Mermin and Wagner[1] rigorously excluded the onset of long-range order in these systems at any nonzero temperature. Nonetheless, numerical analysis of high-temperature series expansions led Stanley and Kaplan[2] to suggest the possible existence of a nonzero pseudo-Curie temperature at which the magnetic susceptibility could become infinite in two-dimensional Heisenberg systems with spin larger than $\frac{1}{2}$.

While the Stanley-Kaplan transition seems now[3] unlikely for two-dimensional Heisenberg models with any spin, extensive work on high-temperature series expansions shows strong evidence for a divergent susceptibility at a finite T_c both in classical[4] and quantum[5] two-dimensional X-Y models.

Quite recently some attempts have been made to study the X-Y system by means of renormalization-group techniques in the manner of Niemeijer and van Leeuwen (NvL).[6,7]

Such an approach, carried out to the second order in a cumulant expansion, allowed Lublin[8] to predict a phase transition in the classical (spin ∞) X-Y model with nearest-neighbor interactions. The existence of a single nontrivial fixed point for the renormalization transformation both in the first- and second-order calculations leads to a conventional description of the critical behavior of the system, with power-law singularities in the thermodynamic quantities.

Even if the critical coupling and critical indices estimated in this way are in qualitative agreement with those predicted on the basis of some high-temperature series investigations,[4] the conventional description of criticality emerging from Lublin's analysis is not compatible with the Kosterlitz and Thouless phenomenological picture[9] of the transition in the classical X-Y system. According to this picture a more complicated fixed-point structure should probably be associated with the transition.

The situation is even less clear as far as the quantum X-Y models are concerned, as, for example, the spin-$\frac{1}{2}$ system.

In fact, the renormalization-group approaches formulated up to now for these systems have not yet given easily interpretable results concerning the existence and nature of the conjectured transition.

Rogiers and Dekeyser[10] and Betts and Plischke[11] have recently introduced a generalization of the NvL method to treat quantum spin systems, and applied it to the plane triangular lattice using both 3-spin[10] and 7-spin[12] cells, and to the square lattice using 5-spin cells.[11]

While in the first-order calculations no fixed point can be found, a nontrivial fixed point appears in the second order for the triangular system. Even in this case, however, the corresponding critical indices and the nearest-neighbor critical couplings are found to be in disagreement with the high-temperature series estimates.[5,13]

Moreover, some of the critical exponents take unphysical values ($\eta < 0$, $\delta < 0$). In our opinion, a possible reason for the last failure can be the fact that in those methods the definition of the transformation

implies an explicit choice of basis in order to preserve the symmetry of the system in spin space.

Such a choice, with the consequence of a possible spurious basis dependence of the results, is not avoidable if one defines the block-spin transformation according to a standard partial-trace procedure, as in the above cases.

In this note we present a quantum-renormalization-group approach in real space, in which the block-spin Hamiltonian is constructed according to a completely different procedure,[14] which in principle allows for a larger freedom in the definition of the transformation and avoids the difficulty of the basis dependence.

Let our system be described by the reduced Hamiltonian

$$H=-\beta\mathcal{H}=\frac{K_1}{2}\sum_{\langle m,n\rangle}(S_m^x S_n^x+S_m^y S_n^y) \quad , \tag{1}$$

where the sum is over nearest-neighbor pairs on a two-dimensional triangular lattice, the Pauli-spin-$\frac{1}{2}$ operators S_m^i $(i=x,y,z)$ are normalized to unity, and $\beta=1/k_B T$, as usual.

Triangular cells are constructed on the lattice, each cell containing three spins $\vec{S}_{l,\alpha}$ where $l=1,2,3$ denotes the spin in the cell and α is a cell index. The state of the system is described as a superposition of products of eigenstates of single-spin operators, e.g., $S_{l,\alpha}^z$. In order to define the renormalization transformation we introduce a new set of spin-$\frac{1}{2}$ operators $\vec{\sigma}_\alpha$, each associated with one of the cells.

A weight operator $P(\{\vec{\sigma}\},\{\vec{S}\})$ is then defined acting on the product space of S and Σ, the spaces of eigenstates of site-spin and cell-spin operators, respectively.

P is chosen in such a way as to satisfy

$$\mathrm{Tr}_\Sigma P(\{\vec{\sigma}\},\{\vec{S}\})=I_S \quad , \tag{2}$$

where Tr_Σ indicates the trace in Σ space and I_S is the identity operator in S space.

Because of (2) we can write the partition function of the system as

$$\begin{aligned} Z&=\mathrm{Tr}_S e^{H(\{\vec{S}\})}=\mathrm{Tr}_\Sigma \mathrm{Tr}_S e^{H(\{\vec{S}\})}P(\{\vec{\sigma}\},\{\vec{S}\}) \\ &=\mathrm{Tr}_\Sigma e^{H'(\{\vec{\sigma}\})} \quad , \end{aligned} \tag{3}$$

where the last equality defines the renormalized Hamiltonian through the relation

$$e^{H'(\{\vec{\sigma}\})}=\mathrm{Tr}_S e^{H(\{\vec{S}\})}P(\{\vec{\sigma}\},\{\vec{S}\}) \quad . \tag{4}$$

The weight operator we use is obtained as a quantum extension of the one first introduced by NvL to treat Ising systems. Namely, the operator is such that it selects a configuration in Σ space in which the αth cell is in an eigenstate of one of the components σ_α^i $(i=x,y,z)$ with eigenvalue ±1, if the configuration of the site spins in S space is an eigenstate of the operator $\mathrm{sgn}\sum_l S_{l\alpha}^i$ with the same eigenvalue.

The operator may thus be written as

$$\begin{aligned} P(\{\vec{\sigma}\},\{\vec{S}\})=\prod_\alpha \frac{1}{2}\Bigg[1&+\sigma_\alpha^x \mathrm{sgn}\sum_l S_{l,\alpha}^x \\ &+\sigma_\alpha^y \mathrm{sgn}\sum_l S_{l,\alpha}^y \\ &+\sigma_\alpha^z \mathrm{sgn}\sum_l S_{l,\alpha}^z\Bigg] \quad , \end{aligned} \tag{5}$$

where the product is extended over all cells in the lattice.

Of course there is a large freedom in the choice of P; in our opinion the above form provides a natural generalization of the majority rule of NvL[6]; manifestly it guarantees the Hermiticity of $H'(\{\vec{\sigma}\})$.

Actual calculations were performed using a cumulant expansion along the lines well established in the literature.[6,7]

After dividing the Hamiltonian into two parts H_0 and V, containing all intracell and intercell interactions, respectively, use is made of Baker-Campbell-Hausdorf[15] formula to write

$$e^{H(\{\vec{S}\})}=e^{H_0(\{\vec{S}\})}e^{W(\{\vec{S}\})} \tag{6}$$

and of a cumulant expansion[16] to obtain from (4)

$$\begin{aligned} H'(\{\vec{\sigma}\})&=\ln \mathrm{Tr}_S e^{H_0}P+\langle W\rangle \\ &\quad+\tfrac{1}{2}(\langle W^2\rangle-\langle W\rangle^2)+\cdots \quad , \end{aligned} \tag{7}$$

where

$$W=V+\tfrac{1}{2}[V,H_0]-\tfrac{1}{12}[2H_0+V,[V,H_0]]+\cdots \quad . \tag{8}$$

The average of a spin operator A is defined according to

$$\langle A\rangle=\frac{\mathrm{Tr}_S e^{H_0(\{\vec{S}\})}A(\{\vec{S}\})P(\{\vec{\sigma}\},\{\vec{S}\})}{\mathrm{Tr}_S e^{H_0(\{\vec{S}\})}P(\{\vec{\sigma}\},\{\vec{S}\})} \quad . \tag{9}$$

The above perturbative algorithm may need to be properly symmetrized in order to yield Hermitian contributions to H' at any given order in K_1.[17]

To first order in K_1 the transformation for the nearest-neighbor coupling turns out to be of the form

$$K_1'=2K_1 f_1^2 \quad , \tag{10}$$

with

$$f_1=(3+4e^{-K_1}+5e^{2K_1})/6z_0 \quad , \tag{11}$$

where

$$z_0=1+2e^{-K_1}+e^{2K_1} \quad . \tag{12}$$

Transformation (10) exhibits a fixed point at

$K_1^* = 0.7463$.

Linearization of (10) at K_1^* yields a thermal eigenvalue $\lambda_T = 1.487$, whereas the magnetic eigenvalue, computed along the usual lines[6,7] by considering a perturbation term of the form $h \sum_{l,\alpha} S_{l\alpha}^x$ in H, has been found to be $\lambda_H = 2.557$.

In this approximation the critical nearest-neighbor[1] coupling is in fairly good agreement with the corresponding quantity as calculated by Betts *et al.*[5] by means of high-temperature expansions, and given as $K_{1c} = 0.667$.[18]

The critical indices, deduced from the above values of λ_T and λ_H, by assuming the validity of scaling relations, are all physical and are reported in Table I. A comparison is made with those predicted by Betts[13] on the basis of scaling by assuming $\gamma = 1.5$ and $\delta = 5$, as estimated from numerical analysis of high-temperature series expansions.

So far, the renormalization group approach seems thus to confirm the existence of a phase transition associated with a single nontrivial fixed point of the transformation, with scaling properties as deduced from series analysis.

A dramatic change in the overall picture is, however, obtained by going further in the cumulant expansion. In fact, in the second-order calculation one gets the renormalization transformation

$$\begin{aligned} K_1' &= 2K_1 f_1^2 + 4K_1^2 f_1 f_2 + 2K_1^2 f_1^2 (f_3 + 1 - 2f_1^2) \\ &\quad + f_1^2 (3K_2 + 2K_3) \ , \\ K_2' &= \tfrac{1}{2} K_1^2 f_1^2 (7f_3 + 1 - 8f_1^2) + f_1^2 K_3 \ , \\ K_3' &= 2K_1^2 (f_3 - f_1^2) \ , \\ L_1' &= K_1^2 (2f_1^4 - f_4^2) + 2f_4^2 L_1 \ , \end{aligned} \tag{13}$$

where f_1 is defined in (11), and

$$f_2 = (1 - e^{2K_1})/2z_0 \ , \tag{14}$$

$$f_3 = 2(e^{2K_1} - e^{-K_1})/3z_0 \ , \tag{15}$$

$$f_4 = (3 + 2e^{-K_1} + e^{2K_1})/3z_0 \ . \tag{16}$$

K_2, K_3, and L_1 are the couplings of the new interactions generated by the transformation. K_2 and K_3 refer to X-Y interactions of the form (1) between second and third neighbors, respectively, while L_1 describes an Ising-like interaction of the form $\frac{1}{2} L_1 \sum_{\langle m,n \rangle} S_m^z S_n^z$ between nearest neighbors.

Contrary to what one would expect, the transformation (13) does not exhibit any nontrivial fixed point: the nontrivial fixed point of the first-order approximation disappears when turning to the next, hopefully better, approximation.

This drastic change of situation is hardly conceivable if, as usually, we think of a transition associated to a single nontrivial fixed point of the renormalization transformation, as the high-temperature series analysis seems to suggest. If this were the case, we would expect some stability of the results, at least in the lowest orders of the cumulant expansion.

To visualize the discrepancy between our second-order results and those of high-temperature series, we have evaluated the dimensionless free energy per spin, f, for the nearest-neighbor model, by iterating the spin-independent part of the transformed Hamiltonian along the lines well established in the literature.[7,19]

The results are plotted in Fig. 1, where they are compared with those obtained from an eleven-term high-temperature expansion.[12]

We see that for relatively low values of K_1, $K_1 \lesssim 0.4$, the two curves agree, while, for higher values of the nearest-neighbor coupling, sizable discrepancies are present, our curve being lower than the series curve.

The absence of a nontrivial fixed point in the second-order calculation could be an indication of the fact that the transition in the spin-$\frac{1}{2}$ X-Y system is of a more complicated nature than that suggested by series expansions and by the above first-order calculations.

For the classical spin-∞ X-Y system there are now[20] indications that the transition may in fact be consistent with the Kosterlitz and Thouless picture.[9]

According to this picture, in which vortex excitations play an essential role, the temperature singularities, when approaching T_c from above, should be of an exponential character, rather than simple power laws.

If a transition of the Kosterlitz and Thouless type is taking place also in the quantum-spin-$\frac{1}{2}$ system, then

TABLE I. Comparison between the critical indices estimated in the present work and those predicted by Betts (Ref. 13) on the basis of high-temperature series analysis.

		γ	δ	Δ	α	ν	η
Present work	First order	1,96	5,88	2,36	−0,76	1,38	0,58
	Second order	...	...	...	...	...	...
High-temperature series expansions		$\frac{3}{2}$	5	$\frac{15}{8}$	$-\frac{1}{4}$	$\frac{9}{8}$	$\frac{2}{3}$

it is sensible that a relatively standard treatment, such as ours, is not adequate to describe correctly the critical behavior. Of course, further investigations are needed to clarify this point.

We believe that our scheme, in particular our choice for P, is useful to describe conventional phase transitions in quantum spin systems. To improve our understanding of the critical behavior in the spin-$\frac{1}{2}$ X-Y model, however, we need a deeper knowledge of its low-temperature and ground-state properties, so that a more specific renormalization transformation may be defined according to the general scheme outlined above.

Finally one more comment on the expression (5) for P seems appropriate.

In the second-order calculation presented above the renormalized Hamiltonian $H'(\{\vec{\sigma}\})$ has the same symmetry properties as $H(\{\vec{S}\})$. In higher-order approximations, however, $H'(\{\vec{\sigma}\})$ will loose the rotational invariance around the z axis in spin space exhibited by (1), since P in Eq. (5) has not its full symmetry.

To avoid this difficulty it is natural to modify the definition of the weight operator in the following way:

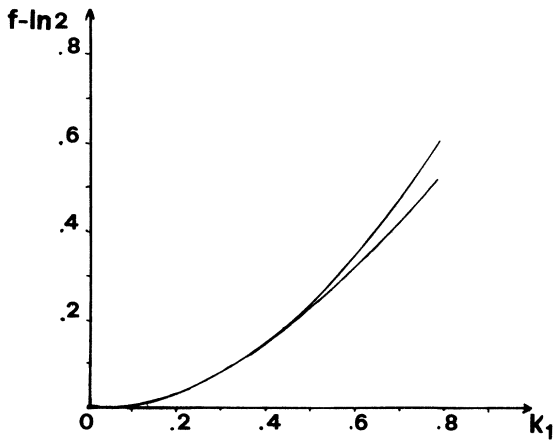

FIG. 1. Dimensionless free energy per spin f (minus ln2). Upper curve: from our second-order transformation. Lower curve: from the eleven-term high-temperature expansion; after Rogiers and Betts (Ref. 12).

$$P(\{\vec{\sigma}\},\{\vec{S}\}) = \frac{1}{2\pi}\int_0^{2\pi} d\phi \prod_\alpha \frac{1}{2}\Bigg[1 + (\sigma_\alpha^x \cos\phi + \sigma_\alpha^y \sin\phi)\,\mathrm{sgn}\sum_l S_{l,\alpha}^x$$

$$+ (\sigma_\alpha^y \cos\phi - \sigma_\alpha^x \sin\phi)\,\mathrm{sgn}\sum_l S_{l,\alpha}^y + \sigma_\alpha^z\,\mathrm{sgn}\sum_l S_{l,\alpha}^z\Bigg] . \tag{5'}$$

Up to second order (5') is completely equivalent to (5), and in general it preserves the symmetry properties of the original Hamiltonian at any order in the cumulant expansion.

Another possibility is that of replacing the sign operators with operators having the transformation properties of the components of a vector in spin space, thus preserving automatically the symmetry at any order. The most simple and obvious example is that of a P operator which induces a linear block-spin transformation.

Work is in progress along these lines to generalize the approach presented above and to investigate the critical properties of other quantum spin systems such as, for example, the Heisenberg model.

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