Possible temperature marginality in the two-dimensional $S = 1/2$ XY model by a linear renormalization transformation

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A real-space linear renormalization transformation is proposed for studying the critical properties of the two-dimensional spin-1/2 XY model on the triangular lattice. The results of various approximations suggest a critical behavior of the same kind as that predicted by other theories and approaches for the classical case. The imposition of marginality for temperature deviations from criticality leads to an almost marginal secondary eigenoperator and to magnetic critical parameters which are not far from currently proposed values for the classical model.

I. INTRODUCTION

The interest in phase transitions in two-dimensional models with continuous symmetry has been growing since it became evident from series expansions¹⁻³ and other approximations⁴ that these models may exhibit singularities in their thermodynamic functions, although they can never develop spontaneous magnetization.⁵ For the XY model, e.g., with which this paper will be concerned, nobody for the moment is doubting that there is some kind of phase transition. There is, however, no unanimity about the nature of this transition, nor about the form of the thermodynamic singularities. Stanley and Kaplan¹ for the Heisenberg model⁶ and later Betts *et al.*³ for the XY model, found some evidence for a power-law behavior of the magnetic susceptibility and other quantities. Kosterlitz and Thouless,^{7,8} on the other hand, predicted from a phenomenological theory for the same model an exponential behavior for the susceptibility, which was confirmed by series analysis of the classical model by Camp and Van Dyke.⁹ Other theories by Berezinskii⁴ and Zittartz¹⁰ also emphasize the fact that there should be a whole range of temperatures for which the free energy is singular, with continuously varying magnetic exponents.

Up to now it has not been possible to reconcile the predictions about the nature of the singularities, as obtained from series analysis of the quantum spin-1/2 XY model, with any of the previously mentioned theories for the classical models. In fact, recently some doubts have been raised¹¹ about the validity of universality with respect to the quantum or classical nature of this model. Arguments in favor of universality, how-

ever, have been given by Goldhirsch *et al.*¹²

In the present situation it is of considerable theoretical interest to apply new techniques to the quantum XY model, independent of the series-expansion method. Recently, the renormalization-group approach has revealed encouraging results in the classical case.¹³⁻¹⁵ It is the purpose of the present paper to show that a quantum renormalization-group method may also yield reasonable results. In addition, these results are not incompatible with some classical predictions.

The real-space renormalization-group approach has already been applied to the spin-1/2 XY model by several authors in different ways, with contradictory results.¹⁶⁻²⁰ All these authors used transformations that are nonlinear in the common renormalization terminology,²¹ what they hoped to be justified by the success of analogous transformations for the Ising model. The fact, however, that the fixed points seem to disappear or appear by changing the kind of approximation or the cell size, indicates that one must be very careful in the choice of transformation. What one needs for making an appropriate choice is a good knowledge of the ground state of the system, as was pointed out by Niemeijer and van Leeuwen.²¹ At present, this is not available for the two-dimensional XY model.

From a general point of view, linear transformations do not require a knowledge of the ground-state properties if one is only interested in the critical properties of the system.²² For this reason we propose to explore more thoroughly this kind of transformation. From a computational point of view, the quantum model that we choose to study is simpler than the classical rotator models,^{13,15} due to the discreteness of the traces

that enter in the calculations.

In working with linear transformations, the price one has to pay for simplicity is the appearance of an extra parameter, which has to be fixed such that the correlation function transforms in a way consistent with the critical properties.²² To make the appropriate choice for this parameter in general requires the use of criteria which cannot be worked out easily, when the approximations are not sophisticated enough. This is the case for the XY model, where the degree of accuracy attained is not very high at present, due to the relative complication of the calculation. Instead of using a self-consistency criterion for completely determining this parameter, we are thus led to look for an external argument to choose its value. In particular, such an argument will be the compatibility of the results obtained with presently accepted properties, as predicted by other approaches for similar systems, namely, the classical rotator models.⁸⁻¹⁰ A common property of the theories for these classical systems is that they imply the presence of a fixed line in the parameter space. Although we cannot hope to reproduce exactly a fixed line within our approximate calculations, we may try to obtain a marginal temperature eigenvalue, which is a local approximation to it. An exact fixed line would probably require us to work with a generalization of the model with extra parameters, and this generalization is not obvious for the moment.¹⁵

After obtaining a marginal (or nearly marginal) temperature eigenvalue, we have to investigate the further critical properties yielded by the transformation and look at their plausibility. This plausibility may be argued from the magnetic eigenvalue λ_h and from the secondary temperature eigenvalue λ_2 . The value of λ_h should be within a physical range and eventually compatible with some predictions for the magnetic exponents in the classical case.⁸⁻¹⁰ Furthermore, the appearance of a secondary marginal or quasimarginal eigenvalue λ_2 is a self-consistency criterion that one should apply in order to determine the parameter in a linear transformation, as discussed by Bell and Wilson.²²

In Sec. II we introduce the linear transformation and explain the different approximations used. The results obtained are then discussed in Sec. III.

II. LINEAR TRANSFORMATION

The XY Hamiltonian that we want to study may be written as

$$-\beta H = \mathcal{K} = K_1 \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad (2.1)$$

where S_j^+ and S_j^- are the spin- $\frac{1}{2}$ raising and lowering operators at the site j on a triangular lattice, and the sum runs over all nearest-neighbor pairs. As usual, the renormalization procedure will produce a whole set of new interactions between next, third, etc., neighbor sites, described by parameters $K_2, K_3, \dots$, and also Ising-like interactions, denoted by $2T_n(S_i^z S_j^z)$, and $n=1, 2, 3, \dots$.

We divide the lattice in the usual way²¹ in triangular cells, numbered by an index α . A new spin- $\frac{1}{2}$ operator $\tilde{\sigma}_\alpha$ is associated with each cell. We then define a linear weight operator P , acting on the product space of S and Σ , the spaces of site-spin and cell-spin operators, respectively:

$$P(\{\tilde{\sigma}\}; \{\tilde{S}\}) = \prod_\alpha \frac{1}{2} [1 + 4p \tilde{\sigma}_\alpha \cdot (\tilde{S}_{\alpha 1} + \tilde{S}_{\alpha 2} + \tilde{S}_{\alpha 3})], \quad (2.2)$$

which has the property

$$\text{Tr}_\Sigma P = I_S, \quad (2.3)$$

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

The renormalization transformation $\mathcal{K} \rightarrow \mathcal{K}'$ is then obtained by exploiting (2.3) in the following way:

$$\begin{aligned} Z &= \text{Tr}_S e^{\mathcal{K}(\{\tilde{S}\})} = \text{Tr}_\Sigma [\text{Tr}_S e^{\mathcal{K}(\{\tilde{S}\})} P(\{\tilde{\sigma}\}; \{\tilde{S}\})] \\ &\equiv \text{Tr}_\Sigma e^{\mathcal{K}'(\{\tilde{\sigma}\})}, \end{aligned} \quad (2.4)$$

where $\mathcal{K}'$ is an interaction Hamiltonian between the cell spins, implicitly defined by the last equation.

One can easily check that this definition of the weight operator is such as to guarantee the usual linear transformation property for the spin-correlation function at large distances.²² In addition, it is the simplest weight operator which preserves spin space symmetry, due to its scalar character.

In order to compute $\mathcal{K}'$ in terms of $\mathcal{K}$, we have to use approximations. In the present case, we applied three different approximations (distinguished by I, II, and III), which are derived from two different expansion schemes. Methods I and II use the conventional cumulant expansion¹⁶⁻²⁰ where, if

$$\mathcal{K} = \mathcal{K}_0 + V, \quad (2.5)$$

one defines an operator W by²³

$$e^{\mathcal{K}_0 + V} = \frac{1}{2} (e^{\mathcal{K}_0} e^W + e^W e^{\mathcal{K}_0}), \quad (2.6)$$

which is satisfied by

$$W = V + \frac{1}{12} [\mathcal{K}_0 - V, [V, \mathcal{K}_0]] + \dots, \quad (2.7)$$

and one obtains from (2.4) by cumulant expansion

$$\mathcal{H}' = \ln \text{Tr}_S(e^{\mathcal{H}_0} P) + \langle W \rangle + \frac{1}{2} \langle (W - \langle W \rangle)^2 \rangle + \dots, \quad (2.8)$$

where for all operators A on S we define

$$\langle A \rangle = (\text{Tr}_S e^{\mathcal{H}_0} P)^{-1} \text{Tr}_S \frac{1}{2} (e^{\mathcal{H}_0} A P + A e^{\mathcal{H}_0} P). \quad (2.9)$$

The difference between methods I and II lies in the treatment of the nearest-neighbor Ising interaction, with strength T_1 . In I this interaction is strictly treated as a driven interaction, which appears in the renormalization as an effect of order K_1^2 , and consequently only the intracell XY interactions are incorporated in the unperturbed part $\mathcal{H}_0$ of the Hamiltonian. In II in contrast, we treat this interaction as a first-order

one from the start, and also put the intracell Ising interactions in $\mathcal{H}_0$. A second-order truncation of the cumulant expansion will in this case also contain terms proportional to T_1^2 , which are not present in method I.

Method III uses the alternative cumulant expansion, based on the time-ordering identity²⁴

$$e^{\mathcal{H}_0 + V} = e^{\mathcal{H}_0} T \exp \left(\int_0^1 d\lambda V(\lambda) \right), \quad (2.10)$$

where T is the "time-ordering" operator with respect to the variable λ and

$$V(\lambda) = e^{-\lambda \mathcal{H}_0} V e^{\lambda \mathcal{H}_0}. \quad (2.11)$$

In this way one obtains, instead of (2.8),

$$\mathcal{H}' = \ln \text{Tr}_S(e^{\mathcal{H}_0} P) + \ln \left(\sum_{n=0}^{\infty} \int_0^1 d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \dots \int_0^{\lambda_{n-1}} d\lambda_n \langle V(\lambda_1) V(\lambda_2) \dots V(\lambda_n) \rangle \right), \quad (2.12)$$

where the mean value is defined as in (2.9), except for the symmetrization. The distinguishing feature of this approach with respect to the previous one, is that here we have in every order a sum over an infinite class of terms which are of higher order than the first expansion.

The Hamiltonian $\mathcal{H}'$ obtained by all three methods is of the same form as the old Hamiltonian, with new interaction parameters. The functional relations between the old and new parameters give the renormalization equations. The general form of these equations is

$$\vec{K}' = \vec{F}(\vec{K}, p), \quad (2.13)$$

where we include also the Ising interaction strengths T_n in the vector $\vec{K}$. The parameter p is still arbitrary for the moment. We now determine its value p_c by imposing the condition that at the fixed point $\vec{K}^*$ of transformation (2.13) there should be a marginal operator, i.e., an eigenvalue $\lambda = 1$ for the linearized renormalization equations.

In practice one works as follows. In trying to solve the fixed-point system $\vec{K}^* = \vec{F}(\vec{K}^*, p)$, one may proceed by eliminating the variables $K_2, K_3, \dots$ and end up with a single equation for K_1 , which can be put in the form

$$K_1' = K_1 f(K_1, p). \quad (2.14)$$

Fixed points are then found for values of K_1 and p that satisfy $f(K_1, p) = 1$. One easily realizes that a marginal operator appears in the linearized transformation, if

$$f' = \frac{\partial f(K_1, p)}{\partial K_1} = 0. \quad (2.15)$$

In Fig. 1 we sketch the typical behavior of this function f in the case of our second-order calculations, for three different values of p . It becomes immediately clear that there is only one value $p = p_c$, for which we can simultaneously satisfy $f = 1$ and $f' = 0$. This determines our fixed point with a marginal eigenvalue.

We performed the calculations up to second order in K_1 (using methods I and III) and to second order in K_1 and T_1 (using method II). We also added to the Hamiltonian a magnetic field interaction

$$-h \sum_j S_j^z, \quad (2.16)$$

in order to obtain the magnetic eigenvalue. In method II, in second order in K_1 and T_1 , this gives rise to a set of ten extra symmetry-breaking interactions besides (2.16)

In first order, methods I and II are equivalent, and fail to yield a marginal eigenvalue, because the function $f(K_1, p)$ is a monotone increasing function of K_1 for all values of p . By applying the criterion $p\lambda_h = 1$,²² implied by hyperscaling, which can be satisfied in this case by choosing $p = 0.380$, one finds $K_c = 0.784$ and critical exponents which are very close to the exponents derived from earlier series analysis³ (e.g., $\gamma \approx 1.5$). A similar thing happens in the first order of method III. This kind of critical behavior, however,

FIG. 1. Sketch of the function $f(K_1, p)$ from Eq. (2.14) vs K_1 , in second-order approximations for three different values of p . In (a) no fixed point can be obtained; in (c) there are two fixed points where $f=1$; in (b) we have a fixed point with a strictly marginal eigenvalue.

seems to be incompatible with the second-order approximations, and also the series analysis is presently being reconsidered.²⁵

In second order, with all our methods, the function $f(K_1, p)$ behaves as sketched in Fig. 1, and we were thus able to determine values for p_c and the parameters $K_1^*, \dots$ for a fixed point with a strictly marginal eigenvalue $\lambda=1$. By linearizing the transformations around these fixed points, we were able to determine the whole set of eigen-

values, including the magnetic one λ_h . Unlike in methods II and III, the marginal eigenvalue in method I does not turn out to be the largest eigenvalue in the even-interaction space. In this case there is another eigenvalue which is slightly higher than unity, and this one must be identified as the principal thermal eigenvalue. By closely studying the flow lines generated by Eq. (2.13), we also determined the critical value K_{1c} for the nearest-neighbor XY model. The results for these second-order calculations are reported in Table I. In all cases, the fixed-point values for T_1^* were around 0.2, and the other parameters were an order of magnitude smaller.

Due to the fact that the Ising-like and XY-like interactions are treated on an equal footing, method II is in principle also suited to determining the other fixed points of the two-dimensional anisotropic Heisenberg model, along with possible cross-over properties. Indeed, one may obtain from them an Ising fixed point ($K_1^*=0$, $T_1^*\approx 0.55$), close to the one obtained by Niemeijer and van Leeuwen,²¹ and also a Heisenberg fixed point ($K_1^*=T_1^*\approx 1.86$). New methods should be developed, however, for studying the eventual critical behavior of the two-dimensional isotropic Heisenberg model, since the fixed-point values are too high to engender confidence in the validity of the cumulant expansion.

III. CONCLUSIONS

The main outcome of our calculations is that we have shown that it is indeed possible to obtain marginality or quasimarginality for the temperature eigenvalue of the two-dimensional XY model with a real-space renormalization method. Furthermore, this marginality comes along with magnetic eigenvalues, which are not incompatible with some predictions for the classical model. Indeed, some authors^{8,13} predict Ising-like values (i.e., $\delta=15$, $\eta=\frac{1}{4}$) for the magnetic exponents at the highest critical temperature, and this would imply $\lambda_h=2.8009$. Of course, in order to get definite evidence for universality between the clas-

TABLE I. Values are given for the following critical parameters: p_c , the weight parameter in the operator (2.2) K_1^* , the fixed point value for the nearest-neighbor XY coupling; K_{1c} , the nearest neighbor XY model critical value; λ_T and λ_2 , the first two temperature eigenvalues of the linearized transformation; λ_h , the magnetic eigenvalue (Ref. 26).

Method	p_c	K_1^*	K_{1c}	λ_T	λ_2	λ_h	$p\lambda_h$
I	0.4054	0.661	0.543	1.149	1	2.806	1.14
II	0.3946	0.721	0.573	1	0.980	$\begin{cases} 3.02 \\ 3.006 \end{cases}$	1.19
III	0.4177	0.779	0.609	1	0.813	2.727	1.14

sical and the quantum case, the calculational effort needed will be several orders of magnitude above the present one.

We note that a marginal temperature eigenvalue, from the point of view of temperature singularities, could be compatible with an exponential behavior, since this corresponds to a limiting case $\nu \rightarrow \infty$.

The fact that $p\lambda_h$ appears to be always relatively close to unity is a further indication of the reliability of the results. We know that a strict imposition of $p\lambda_h = 1$ is not the optimal criterion for determining the parameter p .²²

It is very remarkable that with all three methods we have two temperature eigenvalues which become simultaneously nearly marginal. This supports the interpretation of the observed temperature marginality as a true feature of the criticality of the system. The approximate double marginality is most strongly pronounced with method II, which works in a six-dimensional even-interaction parameter space, compared to the four-dimensional space of the other methods. In this connection, we also mention that the arguments leading to the expectation of a marginal additional eigenvalue that were given by Wilson²⁷ can be straightforwardly generalized to the quantum case.

After the discouraging experiences with the nonlinear transformations for this model,¹⁶⁻²⁰ where the results obtained were highly unstable with respect to changes in the scheme of approximation, the rather good stability that we found here with our three approximations is another argument in favor of the validity of the picture obtained with this linear transformation. In particular, the values for K_{1c} are relatively stable, but at present we are unable to compare these values with specific predictions for the quantum model.²⁵

In order to proceed along these lines, it will be necessary in the future to set up more powerful schemes and approximations, with which the self-consistent criteria might be applied more effectively. We have chosen to apply the external criterion of looking explicitly for a marginal temperature eigenvalue; however, it is very remarkable that this always coincides with the condition of closest approximate fulfillment of a secondary marginality.

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¹H. E. Stanley and T. A. Kaplan, Phys. Rev. Lett. **17**, 913 (1966).

²M. A. Moore, Phys. Rev. Lett. **23**, 861 (1969); M. A. Moore and M. Wortis, Phys. Rev. B **8**, 5205 (1973).

³D. D. Betts, C. J. Elliot, and R. V. Ditzian, Can. J. Phys. **49**, 1327 (1971); D. D. Betts, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. Green (Academic, London, 1974), Vol. 3.

⁴V. L. Berezinskii, Sov. Phys.-JETP **32**, 493 (1970); **34**, 610 (1971).

⁵N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

⁶Evidence for the contrary, however, was given by K. Yamaji and J. Kondo, J. Phys. Soc. Jpn. **35**, 25 (1973).

⁷J. M. Kosterlitz and D. Thouless, J. Phys. C **6**, 1181 (1973).

⁸J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).

⁹W. J. Camp and J. P. Van Dyke, J. Phys. C **8**, 336 (1975).

¹⁰J. Zittartz, Z. Phys. B **23**, 55, 63 (1976).

¹¹A. Luther and D. J. Scalapino, Phys. Rev. B **16**, 1153 (1977).

¹²I. Goldhirsch, E. Levich, and V. Yakhot, Phys. Lett. A **62**, 273 (1977).

¹³J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).

¹⁴V. J. Emery and R. Swendsen, Phys. Rev. Lett. **39**, 1414 (1977).

¹⁵H. J. F. Knops (unpublished).

¹⁶J. Rogiers and R. Dekeyser, Phys. Rev. B **13**, 4886 (1976).

¹⁷D. D. Betts and M. Plischke, Can. J. Phys. **15**, 1553 (1976).

¹⁸J. Rogiers and D. D. Betts, Physica A **85**, 553 (1976).

¹⁹R. Dekeyser, M. Reynaert, and M. H. Lee, Physica B **86-88**, 627 (1977).

²⁰A. L. Stella and F. Toigo, Phys. Rev. B **17**, 2343 (1978).

²¹Th. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. Green (Academic, London, 1976), Vol. 6.

²²For a discussion of the properties of linear transformations, see, T. L. Bell and K. G. Wilson, Phys. Rev. B **11**, 3431 (1975) and K. Subbarao, Phys. Rev. B **13**, 3939 (1976).

²³The essential reason why we define W in this specific way is that this symmetrization of the algorithm avoids the appearance of non-Hermitian terms in $\mathcal{K}'$ after truncation of the cumulant expansion.

²⁴R. C. Brower, F. Kuttner, M. Nauenberg, and K. Subbarao, Phys. Rev. Lett. **38**, 1231 (1977).

²⁵D. D. Betts and J. Rogiers (private communication).

²⁶The reported values of λ_h were calculated to first order in K_1 , except for method II, where in Table I we give two numbers, for the first- and second-order results, respectively.

²⁷K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).