

Phenomenological renormalization-group calculations for 12- and 16-vertex models on a square lattice

J. F. Stilck, M. J. de Oliveira, and S. R. Salinas

Instituto de Física, Universidade de São Paulo, C.P. 20516, 01498 São Paulo, Brazil

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We performed phenomenological renormalization-group calculations for ferroelectric 12- and 16-vertex models on a square lattice with periodic and helical boundary conditions. We considered strips of infinite length and finite widths ($n=1-7,8$, or 9). The extrapolated values for the transition temperature of the 12-vertex model, which has been used for assessing the transition in squaric acid, are lower than the predictions of the Bethe approximation. The estimates for the critical exponent ν do not allow a definite conclusion about its asymptotic behavior, although the Ising value $\nu=1$ seems more plausible. The estimates for the 16-vertex model considered in this paper, which is equivalent to an anisotropic nearest-neighbor Ising model, show an excellent convergence to the exact values. Also, we analyze the finite-size scaling behavior of the critical free energy of both models.

I. INTRODUCTION

The so-called phenomenological renormalization group, proposed by Nightingale a few years ago,¹ has proved to be a powerful method for studying the critical behavior of two-dimensional model systems.² In the present paper we report phenomenological renormalization-group calculations for two vertex models on a square lattice.

We first consider a 12-vertex model associated with the study of the antiferroelectric phase transition in layered hydrogen-bonded crystals of squaric acid.³ At low temperatures, the crystals of squaric acid show an antiferroelectric stacking of ferroelectrically ordered layers.⁴ A ferroelectric 12-vertex model has then been shown to be adequate to account for the ordering in the layers. Although 6-vertex and symmetrical 8-vertex models on a square lattice can be solved exactly, the 12-vertex model does not seem amenable to an exact treatment. On the other hand, in a Bethe-cluster approximation, which gives reasonable results for 6- and 8-vertex models, we have shown the occurrence of a continuous phase transition. It is thus of interest to use more powerful methods to investigate the critical behavior of the 12-vertex model, and to check the predictions of the cluster approximation.

The techniques we use are suitable for assessing the critical behavior of more general vertex models on a square lattice. Thus, we decided to investigate the critical properties of a certain 16-vertex model, which is isomorphous to an Ising model with anisotropic first-neighbor interactions. Since the critical singularities of this Ising model are known exactly, the calculations reported in the present paper are a good test for the reliability of the method. In particular, we reproduce, with somewhat better accuracy, earlier phenomenological renormalization-group results for the anisotropic Ising model.

In Sec. II we define the 12- and 16-vertex models considered in this paper. In addition, we briefly review the equivalence between a 16-vertex model on a square lattice and an anisotropic Ising model with first- and second-

neighbor interactions and four-spin terms. It should be noted that the existence of a phase transition in the ferroelectric 12-vertex model on a square lattice may be established by the application of a Peierls argument.⁵ In Sec. III we recall a theorem by Suzuki and Fisher⁶ concerning the behavior of the zeros of the partition function for vertex models in the complex electric field plane. Arguments based on this theorem indicate that the Bethe approximation may be giving an overestimated value for the critical temperature. This has been confirmed by our renormalization-group calculations for the 12-vertex model.

The numerical estimates for the values of the critical temperature and the exponent ν are given in Sec. IV. The results for the 16-vertex model show an excellent convergence. The convergence of the estimates for the exponent ν of the 12-vertex model are much poorer, although the Ising value $\nu=1$ seems indeed more plausible. Some finite-size scaling data for the critical free energy of these models are analyzed in Sec. V. For the 16-vertex model they exhibit the expected behavior. However, for the 12-vertex model it seems that corrections to scaling are still important even at the highest orders (strips of widths $n=8$ and 9) we were able to consider. A summary and some conclusions are presented in Sec. VI.

II. DEFINITION OF THE MODELS

The vertex configurations of the 16-vertex model may be numbered as shown in Fig. 1. We will be concerned with arrow inversion invariant energy levels e_ξ given by

$$\begin{aligned} e_1=e_2=E_1, \quad e_3=e_4=E_2, \quad e_5=e_6=E_3, \\ e_7=e_8=E_4, \quad e_9=e_{13}=E_5, \quad e_{10}=e_{14}=E_6, \\ e_{11}=e_{15}=E_7, \quad e_{12}=e_{16}=E_8. \end{aligned} \quad (2.1)$$

This vertex model can be converted into an Ising model with first-neighbor, second-neighbor, and four-spin interactions.⁶ Let us define Ising-type variables σ_i on the

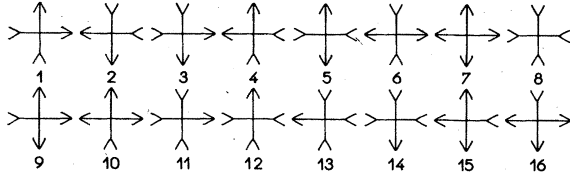


FIG. 1. 16-vertex configurations on a square lattice.

links of the original lattice such that $\sigma_i = 1$ if the arrow on the link points up or rightwards, and $\sigma_i = -1$ if it points down or leftwards. The energy of each vertex may then be written as a function of the four incident Ising spins (see Fig. 2). Therefore, we have

$$E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = -J_0 - (J_1 \sigma_1 \sigma_2 + J_2 \sigma_2 \sigma_3 + J_3 \sigma_3 \sigma_4 + J_4 \sigma_4 \sigma_1) - (J_5 \sigma_1 \sigma_3 + J_6 \sigma_2 \sigma_4) - J_7 \sigma_1 \sigma_2 \sigma_3 \sigma_4, \quad (2.2)$$

where

$$J_0 = -\frac{1}{8} \sum_{i=1}^8 E_i, \quad (2.3a)$$

$$J_1 = \frac{1}{8} [(E_2 + E_3 + E_7 + E_8) + (E_1 + E_4 + E_5 + E_6)], \quad (2.3b)$$

$$J_2 = \frac{1}{8} [(E_2 + E_4 + E_5 + E_8) - (E_1 + E_3 + E_6 + E_7)], \quad (2.3c)$$

$$J_3 = \frac{1}{8} [(E_2 + E_3 + E_5 + E_6) - (E_1 + E_4 + E_7 + E_8)], \quad (2.3d)$$

$$J_4 = \frac{1}{8} [(E_2 + E_4 + E_6 + E_7) - (E_1 + E_3 + E_5 + E_8)], \quad (2.3e)$$

$$J_5 = \frac{1}{8} [(E_3 + E_4 + E_5 + E_7) - (E_1 + E_2 + E_6 + E_8)], \quad (2.3f)$$

$$J_6 = \frac{1}{8} [(E_3 + E_4 + E_6 + E_8) - (E_1 + E_2 + E_5 + E_7)], \quad (2.3g)$$

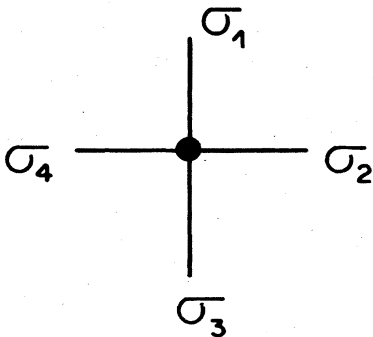


FIG. 2. Numbering scheme for the four links incident on a vertex.

$$J_7 = \frac{1}{8} [(E_5 + E_6 + E_7 + E_8) - (E_1 + E_2 + E_3 + E_4)]. \quad (2.3h)$$

With the particular choice

$$E_1 = -2J(1+R), \quad E_2 = 2J(1+R), \quad (2.4a)$$

$$E_3 = 2J(1-R), \quad E_4 = -2J(1-R), \quad (2.4b)$$

$$E_5 = E_6 = E_7 = E_8 = 0, \quad (2.4c)$$

the 16-vertex model corresponds to an anisotropic Ising model with interactions $J_1 = J_3 = J$ and $J_2 = J_4 = RJ$ between nearest neighbors only. The exact critical temperature of this model is given by⁷

$$\cosh \left[\frac{2J}{kT_c} \right] \cosh \left[\frac{2RJ}{kT_c} \right] = \sinh \left[\frac{2J}{kT_c} \right] + \sinh \left[\frac{2RJ}{kT_c} \right], \quad (2.5)$$

and the correlation-length critical exponent is $\nu = 1$.⁸

The ferroelectric 12-vertex model³ is defined by the energy levels

$$E_1 = 0, \quad E_2 = E > 0, \quad (2.6)$$

$$E_5 = E_6 = E_7 = E_8 = E' > 0, \quad E_3, E_4 \rightarrow \infty.$$

In the Bethe approximation, it exhibits a ferroelectric phase transition of second order.³ By using a rigorous version of the Peierls argument, provided that $E, E' > 0$, it is possible to confirm the existence of this phase transition.⁵

III. BEHAVIOR OF THE ZEROS OF THE PARTITION FUNCTION

Consider ferroelectric vertex models with the lowest energy levels defined by $e_1 = e_2 = E_1$. A theorem proved by Suzuki and Fisher⁶ asserts that the zeros of the partition function lie on a unit circle in a complex $e^{-\beta\epsilon}$ plane, where ϵ is the ordering electric field, provided that the condition

$$e^{-E_1/kT} \geq \sum_{j=2}^{\infty} e^{-E_j/kT} \quad (3.1)$$

is fulfilled. There is thus a limiting temperature T_0 for which the inequality (3.1) turns into an equality. Below T_0 the unit-circle theorem holds for these vertex models.

For a ferroelectric 6-vertex model ($E_1 = 0, E_2 = E_3 = E > 0, E_4, E_5, E_6, E_7, E_8 \rightarrow \infty$), as well as an 8-vertex model ($E_1 = 0, E_2 = E_3 = E > 0, E_4 = E' > 0, E_5, E_6, E_7, E_8 \rightarrow \infty$), for which exact solutions are known,⁸ the limiting temperature T_0 coincides with the transition temperature. Numerical calculations for finite 6-vertex models seem to indicate that the zeros of the partition function actually get off the unit circle for temperatures above T_0 .⁹ On the other hand, the zeros of the partition function for the 16-vertex model (2.4) are known to lie on the unit circle at all temperatures.¹⁰ In this case the limiting temperature T_0 has no special meaning.

There is also a peculiar coincidence between the exact transition temperature T_c of the 6- and 8-vertex models defined above and the corresponding temperatures, $T_{c,B}$, predicted by the Bethe approximation. Since $T_{c,B} > T_0$ for the 12-vertex model, we suspected that the Bethe approximation overestimates the critical temperature. The renormalization-group calculations presented in this paper were undertaken in part to clear up this point.

IV. RENORMALIZATION-GROUP CALCULATIONS

We considered vertex models defined on strips of infinite length and finite width (geometry B , as denoted by Brézin¹¹). The correlation lengths in the longitudinal direction were calculated by a transfer-matrix formalism. The renormalization of the temperature was then obtained via the scaling relation for the correlation length,^{1,11}

$$\frac{\xi_n(z)}{\xi_{n-1}(z')} = \frac{n}{n-1}, \quad (4.1)$$

where z is an activity, and we choose pairs of strips with widths n and $n-1$. The fixed point of the recurrence relation $z' = z'(z)$ gives estimates for the critical activity z_c ,

$$\frac{\xi_n(z_{c,n})}{\xi_{n-1}(z_{c,n})} = \frac{n}{n-1}. \quad (4.2)$$

Estimates for the exponent ν may be calculated by a linearization of the recurrence relation in the neighborhood of the fixed point. We thus have

$$\nu_n = \frac{\ln[\xi_n(z_{c,n})/\xi_{n-1}(z_{c,n})]}{\ln[n/(n-1)]} - 1, \quad (4.3)$$

where $\dot{\xi} \equiv d\xi/dz$.

Two sequences of estimates were obtained: (i) for periodic boundary conditions, and with the usual definition of the transfer matrix for vertex models;¹² (ii) for helical boundary conditions. Details regarding the definitions and calculation of the transfer matrices, as well as the determination of the correlation lengths, are given in the Appendixes. In general, the transfer matrices of vertex models with periodic boundary conditions are not Hermitian. However, it is remarkable that the ferroelectric 12-vertex model obeys the conditions $E_3 = E_4$ and $E_5 = E_7$, which are sufficient to ensure that the corresponding transfer matrix is Hermitian.

In Table I we display estimates of $z_c = \exp(-E/kT_c)$ and the exponent ν for the 12-vertex model with periodic boundary conditions, for six different values of the ratio $p = E/E'$. In the limit $p \rightarrow 0$, the 12-vertex model reduces to a 4-vertex model, and $z_c = 1$.³ The values of $z_{c,B} = \exp(-E/kT_{c,B})$, corresponding to the Bethe approximation, and of $z_0 = \exp(-E/kT_0)$, are also given in Table I. It is apparent that, in general, $T_0 < T_c < T_{c,B}$ for the 12-vertex model. Estimates for this model under helical boundary conditions are shown in Table II. In Figs. 3(a) and 3(b) the estimates for the 12-vertex model are displayed graphically.

The estimates for the 16-vertex model, which is equivalent to an anisotropic Ising model, are given in Tables III and IV, for periodic and helical boundary con-

TABLE I. Estimates of the critical activity z_c and the exponent ν for the ferroelectric 12-vertex model with periodic boundary conditions. The subscript n refers to a comparison between two models with widths n and $n-1$. Values of $z_{c,B} \equiv \exp(-E/kT_{c,B})$ and $z_0 = \exp(-E/kT_0)$ are also given. The parameter p is given by the ratio E/E' , with the energy levels defined in Eq. (2.6).

n	$z_{c,n}$	ν_n	n	$z_{c,n}$	ν_n
$p=2, z_{c,B}=0.17157, z_0=0.05572$			$p=1, z_{c,B}=\frac{1}{3}, z_0=0.2$		
3	0.15711	1.322	3	0.28363	1.057
4	0.12713	1.036	4	0.29328	0.958
5	0.11242	0.970	5	0.28704	0.928
6	0.10525	0.959	6	0.28013	0.928
7	0.10171	0.964	7	0.27519	0.937
8	0.09991	0.971	8	0.27207	0.948
$p=\frac{1}{2}, z_{c,B}=\frac{1}{2}, z_0=0.39039$			$p=\frac{1}{3}, z_{c,B}=0.58975, z_0=0.5$		
3	0.42472	0.926	3	0.50742	0.895
4	0.45779	0.874	4	0.54334	0.843
5	0.46783	0.846	5	0.55938	0.808
6	0.46903	0.844	6	0.56563	0.793
7	0.46740	0.856	7	0.56736	0.796
8	0.46524	0.875	8	0.56715	0.809
$p=\frac{1}{4}, z_{c,B}=0.64780, z_0=0.57195$			$p=\frac{1}{5}, z_{c,B}=0.68914, z_0=0.62340$		
3	0.56410	0.887	3	0.60625	0.887
4	0.59872	0.830	4	0.63868	0.825
5	0.61657	0.792	5	0.65671	0.784
6	0.62536	0.768	6	0.66669	0.756
7	0.62930	0.760	7	0.67197	0.740
8	0.63071	0.764	8	0.67454	0.736

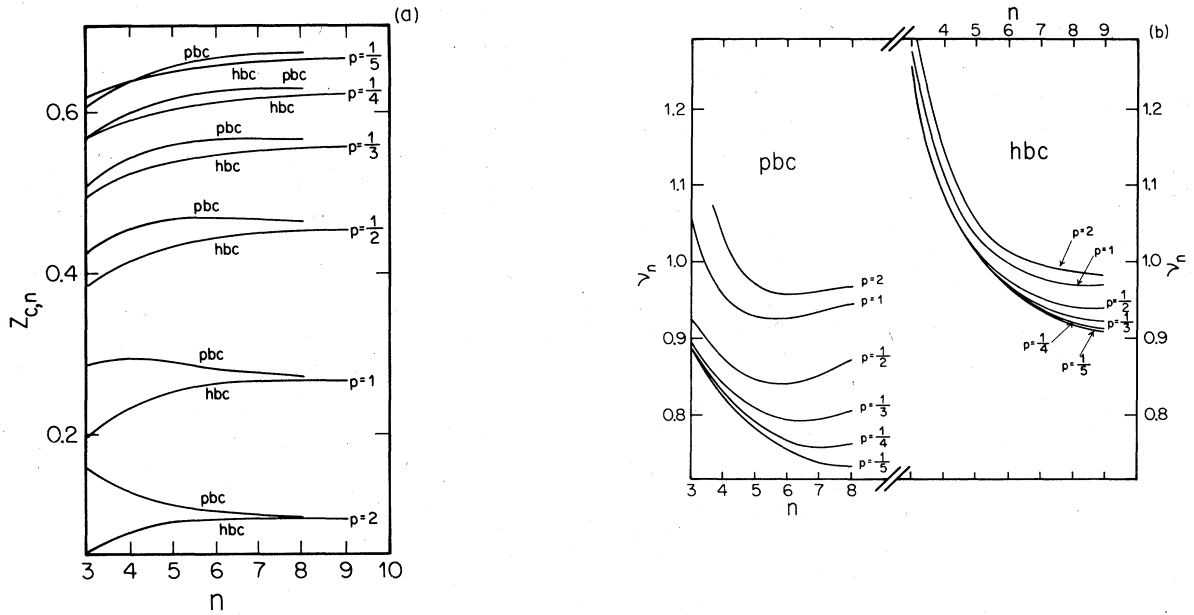


FIG. 3. Graphs of the estimates for z_c and ν , as a function of the widths n , of the ferroelectric 12-vertex model: (a) estimates of z_c , with periodic (pbc) and helical (hbc) boundary conditions (see Tables I and II); (b) estimates of ν with periodic boundary conditions (see Table I) and with helical boundary conditions (see Table II). We display results for several values of the parameter $p = E/E'$.

TABLE II. Estimates of the critical activity z_c and the exponent ν for the ferroelectric 12-vertex model with helical boundary conditions.

n	$z_{c,n}$	ν_n	n	$z_{c,n}$	ν_n
$p = 2$			$p = 1$		
3	0.052 95	1.331	3	0.194 17	1.277
4	0.078 34	1.151	4	0.233 39	1.118
5	0.090 24	1.063	5	0.252 04	1.040
6	0.094 99	1.022	6	0.260 68	1.003
7	0.096 75	1.004	7	0.264 56	0.986
8	0.097 35	0.996	8	0.266 23	0.978
9	0.097 52	0.993	9	0.266 92	0.980
$p = 1/2$			$p = 1/3$		
3	0.382 99	1.251	3	0.492 62	1.249
4	0.418 70	1.100	4	0.522 47	1.097
5	0.436 64	1.022	5	0.537 79	1.019
6	0.446 30	0.982	6	0.546 53	0.976
7	0.451 66	0.961	7	0.551 81	0.951
8	0.454 67	0.951	8	0.555 10	0.938
9	0.456 36	0.948	9	0.557 18	0.931
$p = 1/4$			$p = 1/5$		
3	0.564 95	1.244	3	0.616 83	1.245
4	0.590 30	1.097	4	0.638 82	1.098
5	0.603 44	1.019	5	0.650 28	1.019
6	0.611 16	0.974	6	0.657 12	0.974
7	0.616 03	0.949	7	0.661 53	0.846
8	0.619 22	0.932	8	0.664 51	0.929
9	0.621 35	0.923	9	0.666 59	0.918

TABLE III. Estimates of $z_c = \exp(-J/kT_c)$ and the exponent ν for the particular 16-vertex model defined by Eqs. (2.4), with periodic boundary conditions. J and RJ are the exchange parameters of the equivalent anisotropic Ising model on the square lattice. The exact values of z_c and ν are also given.

n	$z_{c,n}$	ν_n
$R=1, z_c=0.643\ 60, \nu=1$		
3	0.639 69	1.039
4	0.642 05	1.021
5	0.642 94	1.013
6	0.643 17	1.008
7	0.643 33	1.006
$R=2, z_c=0.737\ 36, \nu=1$		
3	0.735 07	1.042
4	0.736 49	1.025
5	0.736 94	1.017
6	0.737 12	1.013
7	0.737 21	1.010

ditions, respectively. These estimates, as well as the exact values of $z_c = \exp(-J/kT_c)$ and ν , are plotted in Figs. 4(a) and 4(b).

The estimates for the 16-vertex model converge to their asymptotic values faster than the corresponding ones for the 12-vertex model. As a matter of fact, for the 12-vertex model, the curves $z_{c,n}$ versus n and ν_n versus n display, in some cases, a nonmonotonic behavior. We thus conclude that the estimates for the 12-vertex model, up to the orders we considered, have not reached the regime where their convergence is governed by the leading irrelevant-variable scaling exponent.¹³ This makes it difficult to devise a reliable extrapolation scheme for the estimates, particularly for those of the exponent ν . Therefore, it remains an open question whether ν has a unique value for the 12-vertex model. We recall that calculations for the 8-vertex model indicate that the phenomenological renormalization-group technique may give good results

TABLE IV. Estimates of z_c and ν for the 16-vertex model defined by Eqs. (2.4) with helical boundary conditions.

n	$z_{c,n}$	ν_n
$R=1$		
3	0.624 85	1.060
4	0.635 62	1.038
5	0.639 54	1.026
6	0.641 27	1.018
7	0.642 14	1.014
8	0.642 63	1.010
9	0.642 92	1.008
$R=2$		
3	0.716 22	1.160
4	0.726 43	1.105
5	0.730 77	1.077
6	0.732 99	1.059
7	0.734 26	1.048
8	0.735 05	1.040
9	0.735 58	1.034

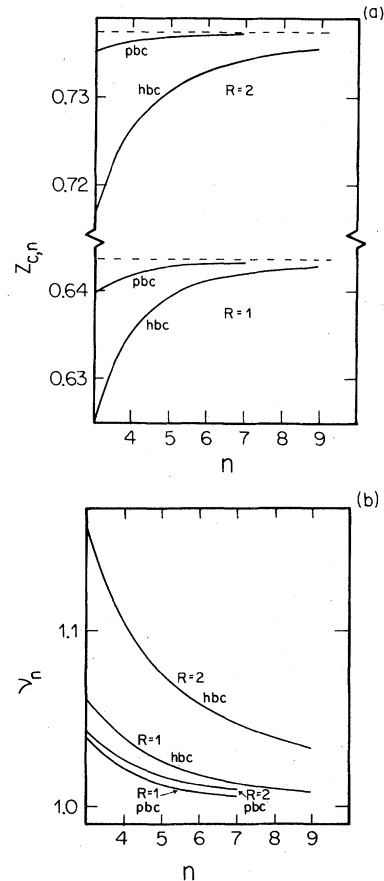


FIG. 4. Graphs of the estimates, as a function of the widths n , for the particular 16-vertex model defined by Eqs. (2.4) (see Tables III and IV): (a) estimates of z_c , with periodic (pbc) and helical (hbc) boundary conditions; (b) estimates of ν , with periodic (pbc) and helical (hbc) boundary conditions.

TABLE V. Three-point fits for the estimates in Table III with functions of the form $A + Bn^{-x}$, associated with three consecutive widths, $n, n+1$, and $n+2$.

n	A	B	x
$R=1, z_c$			
3	0.643 58	-0.140 20	3.2656
7	0.643 59	-0.134 64	3.2312
5	0.643 59	-0.130 62	3.2093
$R=1, \nu$			
3	1.000 18	0.410 17	2.1395
4	0.999 10	0.359 04	2.0073
5	1.001 92	0.803 76	2.6461
$R=2, z_c$			
3	0.737 33	-0.101 17	3.4600
4	0.737 34	-0.092 62	3.3859
5	0.737 35	-0.085 78	3.3309
$R=2, \nu$			
3	1.003 63	0.344 89	1.9857
4	1.002 89	0.318 52	1.9042
5	1.002 32	0.289 28	1.8211

for systems with nonuniversal critical behavior.¹⁴ Nevertheless, some fits of our estimates for the 12-vertex model, with the allowance of logarithmic corrections, are consistent with the assumption that it has a universal critical behavior, with $\nu=1$. These fits, however, are by no means definitive.

The estimates for the 16-vertex model behave as expected. In Table V we present results of three-point fits of functions of the form $A+Bn^{-x}$ to the estimates. They seem to be consistent with $x_z=3$ for $z_{c,n}$ and $x_\nu=2$ for ν_n . This supports the scaling relation^{13,15}

$$x_z - x_\nu = 1/\nu. \quad (4.4)$$

The exponents governing the convergence of our estimates seem to be given by the usual values obtained in the Onsager formulation of the Ising model.¹⁵ The amplitudes, however, are different. Our estimates converge more rapidly to their asymptotic values than the corresponding ones obtained via the Onsager formulation of the transfer matrix.^{1,16} Also, due to the way we formulate the Ising model, even in the anisotropic case ($R \neq 1$), the direction in which the correlation length is calculated is equivalent to the direction along which the widths of the strips are measured.

V. FINITE-SIZE SCALING OF THE FREE ENERGY

According to finite-size scaling arguments, the critical free energy per vertex is asymptotically given by

$$f_n \cong A + Bn^{-d}, \quad (5.1)$$

where d is the spatial dimensionality of the lattice.¹⁷ In order to verify Eq. (5.1), we calculated the critical free energies f_n given by

$$f_n = -kT_c \frac{\ln[Z_n(T_c)]}{NJ} \quad (5.2)$$

for the 16-vertex Ising model with strips of width n (for the 12-vertex model, J should be replaced by E).

In Table VI we give values of the critical free energy f_n for Ising models with width n and periodic boundary conditions. Three-point fits of functions of the form $A+Bn^{-x}$ to these values seem to support the prediction $x=2$ (see Table VII). In these calculations, the values of f_n converge faster than in the usual Onsager formulation of the Ising model. For the isotropic case, $B \cong 1.188\ 142$ in the Onsager formulation, whereas $B \cong 0.557$ in our calculations.

TABLE VI. Values of the critical free energy for the 16-vertex Ising model with periodic boundary conditions.

n	$f(0, n^{-1})$	n	$f(0, n^{-1})$
$R=1$		$R=2$	
2	-4.359 35	2	-6.484 24
3	-4.283 47	3	-6.381 93
4	-4.255 84	4	-6.345 00
5	-4.242 83	5	-6.437 69
6	-4.235 71	6	-6.318 23
7	-4.231 39	7	-6.312 50

TABLE VII. Three-point fits with functions of the form $A+Bn^{-x}$ for the critical free energies of Table VI.

n	A	B	x
$R=1$			
2	-4.217 59	-0.525 39	1.8899
3	-4.218 72	-0.542 08	1.9342
4	-4.219 17	-0.557 94	1.9637
5	-4.219 17	-0.557 62	1.9633
$R=2$			
2	-6.294 73	-0.714 42	1.9145
4	-6.295 98	-0.733 61	1.9517
4	-6.296 32	-0.746 32	1.9692
5	-6.296 44	-0.753 79	1.9776

Similar calculations for the 12-vertex model are not so accurate since the exact critical temperature is not known. Values for f_n obtained using the estimates for z_c of the preceding section provided nonmonotonic estimates for B and x . We are thus led to the conclusion that the asymptotic regime has not been attained and, therefore, corrections to scaling become relevant.

VI. CONCLUDING REMARKS

We performed phenomenological renormalization-group calculations and used finite-size scaling arguments to analyze the critical behavior of 12- and 16-vertex models on a square lattice.

For a particular 16-vertex model, which is equivalent to the anisotropic Ising model with first-neighbor interactions, the renormalization-group calculations produced quite accurate results both for the critical temperature and for the critical exponent $\nu=1$. Also, the behavior of the estimates as a function of the widths of the strips used in the calculations is well described by the expected asymptotic scaling law. It is thus possible to devise a reliable extrapolation scheme. We obtain extrapolated values with relative errors of about 0.001% for T_c and 0.1% for ν . The critical free energies of the strips are also in good agreement with the expected asymptotic behavior for the 16-vertex Ising model.

The results for the ferroelectric 12-vertex model are not so well behaved. In several cases, the estimates for z_c and ν show a nonmonotonic dependence on the width of the strips. This is an indication that the asymptotic regime has not been reached up to the widths we considered. Nevertheless, the estimates for z_c are sufficiently accurate to allow the conclusion that the Bethe approximation for the 12-vertex model leads to an overestimated value of the critical temperature. Although we believe that the correlation-length exponent for the 12-vertex model is equal to the Ising value, $\nu=1$, other values of ν , or even a nonuniversal behavior of the model, cannot be ruled out by our estimates.

All calculations were performed for vertex models defined on strips of widths up to $n=7$ (16-vertex model with periodic boundary conditions), $n=8$ (12-vertex model with periodic boundary conditions), and $n=9$ (heli-

cal boundary conditions). We believe that it would be feasible to consider larger strips, particularly in the case of helical boundary conditions, and to use better numerical methods for obtaining the two largest eigenvalues of the transfer matrix (we used a variation of the power method¹⁸). Nevertheless, since the estimates seem to converge slowly, it is doubtful whether this improvement would provide a definitive answer about the value of the critical exponent ν for the 12-vertex model.

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APPENDIX A: TRANSFER MATRIX FOR VERTEX MODELS WITH HELICAL BOUNDARY CONDITIONS

Consider a vertex model defined on a strip of width n and length m . The total number of vertices will be $N=nm$. Usually,¹² the transfer matrix with periodic boundary conditions is defined by

$$T(\varphi, \varphi') = \sum_{\theta} \exp \left[-\frac{E_n(\varphi, \theta, \varphi')}{kT} \right], \quad (\text{A1})$$

where φ and φ' label the configurations of two disjoint sets of n vertical bonds, and θ labels the configuration of the n horizontal bonds between them (see Fig. 5). The value of $E_n(\varphi, \theta, \varphi')$ is given by the sum of the contributions of the n vertices whose configurations are defined by φ , θ , and φ' . In the limit $m \rightarrow \infty$, the partition function is asymptotically given by

$$Z_{nm} \simeq \lambda_1^m, \quad (\text{A2})$$

where λ_1 is the largest eigenvalue of the matrix $T(\varphi, \varphi')$. Also, the correlation length associated with the vertical-bond-vertical-bond correlations in the longitudinal direction is given by

$$\xi = [\ln(\lambda_1/\lambda_2)]^{-1}, \quad (\text{A3})$$

where λ_2 is the second-largest eigenvalue. Alternatively, we may define the vertex model on a strip where the horizontal bonds lay along a helix. These boundary conditions were used by Kramers and Wannier for the Ising model.¹⁹ We may then number the vertices, as well as the vertical and horizontal bonds, along the helix, as depicted in Fig. 6, and associate an Ising spin σ_v (σ_h) with each vertical (horizontal) bond according to the conventions of Sec. II. The Hamiltonian may then be written as

$$\mathcal{H} = \sum_{i=1}^N E(\sigma_{v_i}, \sigma_{h_{i-1}}, \sigma_{v_{i-n}}, \sigma_{h_i}), \quad (\text{A4})$$

with

$$\sigma_{v_0} = \sigma_{v_N}, \sigma_{v_{-1}} = \sigma_{v_{N-1}}, \dots, \sigma_{v_{1-n}} = \sigma_{v_{N-n+1}}, \quad (\text{A5a})$$

and

$$\sigma_{h_0} = \sigma_{h_N}. \quad (\text{A5b})$$

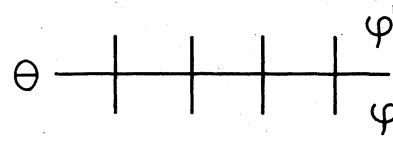


FIG. 5. Two rows of vertical bonds and a row of horizontal bonds for a vertex model with periodic boundary conditions and width $n=4$.

The partition function is given by

$$Z_n = \sum_{\{\sigma_v\}} \sum_{\{\sigma_n\}} \prod_{i=1}^N \exp[-E(\sigma_{v_i}, \sigma_{h_{i-1}}, \sigma_{v_{i-n}}, \sigma_{h_i})/kT]. \quad (\text{A6})$$

Let us now group the bonds in N sets of $n+1$ bonds defined by

$$S_i = \{\sigma_{v_{i-1}}, \sigma_{v_{i-2}}, \dots, \sigma_{v_{i-n}}, \sigma_{h_{i-1}}\}, \quad (\text{A7})$$

with $i=1, 2, \dots, N$, and $S_{N+1}=S_1$. The configurations of each set may be labeled by an index $\varphi_i=1, 2, \dots, 2^{n+1}$, and the partition function (A6) may be rewritten as

$$Z_n = \sum_{\varphi_1=1}^{2^{n+1}} \sum_{\varphi_2=1}^{2^{n+1}} \dots \sum_{\varphi_N=1}^{2^{n+1}} \prod_{i=1}^N T(\varphi_i, \varphi_{i+1}) = \text{Tr } \underline{T}^N, \quad (\text{A8})$$

where

$$T(\varphi_i, \varphi_{i+1}) = \begin{cases} 0 & \text{if } \varphi_{i+1} \text{ is not compatible with } \varphi_i, \\ \exp[-E(v_i, h_{i-1}, v_{i-n}, h_i)/kT] & \text{if they are compatible.} \end{cases} \quad (\text{A9})$$

It should be remarked that the transfer matrix will be sparse. There will be, at most, four nonzero elements in each line. In the limit $m \rightarrow \infty$, the partition function and the correlation length will be given by

$$Z_N \cong \Lambda_1^N, \quad (\text{A10})$$

and

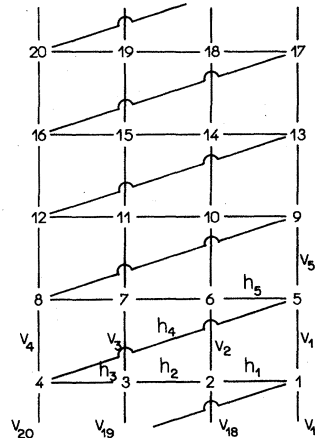


FIG. 6. Lattice with $n=4$ and $m=6$ under helical boundary conditions.

$$\xi \simeq [\ln(\Lambda_1/\Lambda_2)^n]^{-1}, \quad (\text{A11})$$

where Λ_1 and Λ_2 are the largest and the second-largest eigenvalues of the transfer matrix, respectively.

**APPENDIX B: BLOCK DIAGONALIZATION
OF THE TRANSFER MATRIX OF
VERTEX MODELS WITH PERIODIC BOUNDARY
CONDITIONS**

Before performing numerical calculations with periodic boundary conditions we used symmetry properties to alge-

braically block-diagonalize the transfer matrix. As may be seen in Appendix A, the states which define the transfer matrix are invariant under rotations of $2\pi/n$, as well as under the inversion of the arrows. Therefore, the symmetry group to be considered is $C_{n,h} = C_n \otimes S_2$. First, we obtained the character table of this group, with n between 2 and 8. We then constructed the unitary matrix \underline{S} in order to transform \underline{T} into $\underline{T}' = \underline{S} \times \underline{T} \times \underline{S}^\dagger$. The computational effort in doing these calculations grows very fast with n , and this imposed severe limitations on the widths we were able to consider.

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