Corrections to scaling at two-dimensional Ising transitions

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We investigate the completeness of the set of irrelevant critical exponents predicted by conformal invariance, particularly the question of whether the set of operators in the conformal block is complete in general, or only in a subspace of the critical hypersurface. The leading correction-to-scaling exponent is determined numerically at the critical points of some versions of the two-dimensional Ising model that enhance vacancy excitations: the antiferromagnetic Ising model in a magnetic field and the Blume-Capel model. The presence of corrections to scaling with the vacancy exponent $y_{\text{vac}}=-\frac{4}{3}$ would be consistent with conformal invariance, but would contradict completeness of the closed operator algebra. Only corrections to scaling with an irrelevant critical exponent $y_{\text{ir}}=-2.0$ are found, consistent with completeness. However, an investigation of the random-cluster-model representation of the $q=2+\epsilon$ state Potts model shows that a vacancy correction to scaling with exponent $y_{\text{vac}}=-\frac{4}{3}$ appears. The correction is of order ϵ: its amplitude vanishes in the Ising case $q=2$.

I. INTRODUCTION

The dominant scaling properties of a number of two-dimensional (2D) phase transitions have been determined in recent years, but questions remain about the correction-to-scaling exponents. Guided by the recent theoretical results obtained from conformal invariance and extended scaling, we identify three classes of irrelevant operators, associated with corrections to scaling. We study these corrections numerically by means of finite-size scaling in infinitely long strips of some critical models in the Ising universality class: the antiferromagnetic (AF) Ising model in a magnetic field, the Blume-Capel model, and the random-cluster representation of the q-state Potts model with $q \approx 2$. These are models where corrections to scaling due to the irrelevant so-called vacancy operator can be expected.

Before formulating the question we address in this paper in more detail, it is useful to summarize and compare two general methods that have been used to determine the exact values of critical exponents of 2D models: one uses conformal invariance and the other extended scaling.

In the conformal invariance method one assumes that at criticality correlation functions are invariant under conformal transformations (for details see, e.g., papers by Belavin *et al.*,[1] Friedan *et al.*,[2] and Cardy[3]). This leads to the Virasoro algebra. Its central charge c serves as the parameter characterizing universality classes. At each value of c an infinite set of so-called primary operators, which obey conformal invariance, is constructed. These operators are labeled by integers p and q as $\Phi_{p,q}$ and have scaling dimension

$$\Delta_{p,q}=\frac{(np-mq)^2-(n-m)^2}{4nm} ,$$

where the integers n and m relate to the central charge c by

$$c=1-6(n-m)^2/nm .$$

The critical dimension x_k of the kth observable operator O_k (energy, magnetization, etc.) satisfies $x_k=\Delta_{p_k,q_k}+\Delta_{p_{k'},q_{k'}}$. The primed and unprimed labels are equal for rotationally invariant O_k. For these rational values of c, the operators inside the so-called conformal block with $0<p<m$ and $0<q<n$ form a closed operator product algebra.[1] The condition of unitarity selects a smaller subset of rational values of c, corresponding to[2] $n=m+1$, also known as the "main series."

The conformal invariance method is very general in nature; it predicts sets of critical exponents without making reference to microscopic models. However, it has not been possible yet to identify which value of c corresponds to which universality class, besides by recognition, i.e., by comparison with the values of critical exponents known from other methods. For example, $c=\frac{1}{2}$ turns out to correspond to the Ising, and $c=\frac{4}{5}$ to the 3-state Potts universality class. In addition to the values of the critical exponents, also the universal amplitudes in the finite-size scaling behavior of, e.g., the free energy, correlation length, and surface tension have been determined as functions of c (see, e.g., Refs. 3–5).

The second method of deriving sets of critical exponents, the so-called extended scaling method, is less general but it has the advantage of being microscopic in nature; it predicts which exponents belong to specific excitations in specific models. This method has proved to be very valuable for the determination of the exact values of the critical exponents of many 2D universality classes in recent years, (see, e.g., den Nijs,[6] Knops,[7] and

Nienhuis[8] for a review). The extended scaling method works as follows: a specific model, which is representative for a specific universality class, is shown to be related to the Gaussian model by construction of a mapping into a Coulomb-gas representation. The universality class is then characterized by the value of the Gaussian coupling constant K_G (i.e., the point along the Gaussian fixed line to which the critical point flows under renormalization), and the operators are characterized by their spin-wave and vorticity numbers. The disadvantage of this microscopic approach, although it works in general, is that a new mapping has to be found for each specific model under consideration.

The question we address in this paper is whether the set of operators under which the conformal algebra closes, the set inside the conformal block, is complete. Conformal invariance suggests, but does not imply, that only the operators in the conformal block are realized in a universality class. If this is the case, then not only the asymptotic scaling behavior, but also the entire structure of all corrections to scaling would be known exactly and be simple. For example, in the Ising universality class only corrections to scaling with critical dimension $x=n$ (with n an integer >2) would be possible if the symmetry-breaking field is absent.

On the other hand, the extended scaling method does not suggest completeness of the conformal block. For example, in the Ising universality class it suggests the presence of corrections to scaling due to so-called vacancy excitations,[9] with critical dimension $x_{\rm vac}=\frac{10}{3}$ which can be identified with the operator $\Phi_{3,1}$, which lies outside the conformal block for $c=\frac{1}{2}$ (the Ising model).

More generally, one would expect that microscopic models and experimental realizations include various types of short distance aspects that do not obey conformal invariance and give rise to nonconformal corrections to scaling, with arbitrary exponents. Such a model or experimental system would obey conformal invariance only in the scaling limit, i.e., only its fixed-point Hamiltonian would be conformally invariant.

It is useful to distinguish between three conceivable types of irrelevant operators:

(i) The irrelevant operators inside the conformal block. We will denote them by an index 1, $O_{{\rm ir},1}$. Some of the so-called primary operators have irrelevant exponents. Moreover, conformal theory associates to each primary operator $\Phi_{p,q}$ an infinite tower of gradient operators with critical exponents $\Delta_{p,q}+k$ (with k an integer equal to the order of the derivative). It is probably correct to classify these gradient operators as redundant,[10] since the type of corrections to scaling they give rise to in the free energy are of the same nature as those generated by a nonlinear transformation of the scaling fields.

(ii) At each value of the central charge leading to a closed subalgebra, there are, in principle, infinitely many more operators that obey conformal invariance, but are outside the conformal block of operators that form the closed operator product algebra. The presence of corrections to scaling from these $O_{{\rm ir},2}$ operators would indicate that the model Hamiltonian obeys conformal invariance, but that its closed operator product algebra is not complete. Selection rules can take care that these operators do not couple via operator product expansions to relevant operators $\Delta_{p,q}<1$ outside the conformal block.

(iii) Nonconformal irrelevant operators $O_{{\rm ir},3}$ representing nonconformal short distance aspects in the Hamiltonian, with unknown critical dimensions form our third class.

In the Ising universality class ($c=\frac{1}{2}$) the conformal block includes only three primary operators: the trivial operator with critical dimension $x=2$, the magnetic field operator O_H with $x_H=\frac{1}{8}$, and the energy operator O_T with $x_T=1$. Therefore, in the absence of the symmetry breaking field, only corrections to scaling due to the gradients of the energy and trivial operator, with integer critical dimensions $x=n$ ($n>2$), are consistent with completeness of the closed operator product expansion algebra.

The operator $\Phi_{3,1}$ of the conformal theory can be recognized as the vacancy operator in the extended scaling literature. At $c=\frac{1}{2}$ it has critical dimension $x_{\rm vac}=\frac{10}{3}$, but does not belong to the conformal block. So it is of type 2 and its presence in the Ising model would indicate that the conformal block is incomplete. In this paper we focus on this operator because we know from extended scaling the topological aspect in the spin configurations that are associated with it, and therefore we also know how to modify the Ising model to introduce or to enhance vacancy excitations.

Vacancy excitations play an important role in our understanding of the crossover of the order-disorder transition in the q-state Potts model from critical to first-order at $q=4$ as explained by Nienhuis *et al.*,[9] and also in the extended scaling derivation of the critical exponents of the Potts model given by den Nijs[6,11] and by Nienhuis.[12] This operator must be present in the random-cluster model, which is a formulation of the Potts model for continuous values of the number q of spin states. Indeed at integers values of $q>2$ (and also along the tricritical branch of the Potts model) the vacancy operator becomes part of the conformal block. In extended scaling it is allowed that the amplitude of the vacancy operator vanishes accidentally at $q=2$, but one would expect that its correction to scaling contributions show up at least in some generalizations of the nearest-neighbor Ising model.

Exact solutions like Onsager's solution[13] of the Ising model and Baxter's solution[14] of the hard hexagon model indicate completeness of the conformal block. As far as we know, the corrections to scaling in all exactly soluble models can be explained from irrelevant operators of type 1. For example, in Onsager's solution of the Ising model the vacancy exponent $x_{\rm vac}=\frac{10}{3}$ is absent. On the other hand, completeness of the set of operators in the conformal block, which greatly reduces the pertinent operator product algebra, might be essential to exact solubility.

In the special case of the nearest-neighbor Ising model the evidence for completeness is even stronger. At its critical point also the scaling behavior of the correlation functions is known exactly (see, e.g., Kadanoff and Ceva[15]). The set of these correlation functions is believed to be complete. It contains critical exponents of type 1 only. Therefore, spin interactions such as next-nearest-neighbor interactions, four-spin interactions, and also a staggered magnetic field, seem to be part of the closed operator algebra. This suggests that at least in the local neighborhood of the nearest-neighbor Ising model the closed operator product algebra remains complete.

Figure 1 summarizes the problem we want to answer. It shows a schematic phase diagram. The vertical plane spanned by the scaling field $u_{ir,1}$ and u_{rel} represents the subspace of conformally invariant interactions inside the conformal block. The scaling field u_{rel} represents the relevant interactions, such as the temperature. The scaling field $u_{ir,1}$ represents irrelevant interactions inside the conformal block, such as the gradient followers of the energy operator (type 1). Point F represents the fixed point. If the gradient operators are indeed redundant, then F will move inside the critical subspace spanned by the type-1 irrelevant interactions, by means of a nonlinear transformation of the scaling fields. The second irrelevant scaling field $u_{ir,2}$ represents interactions that

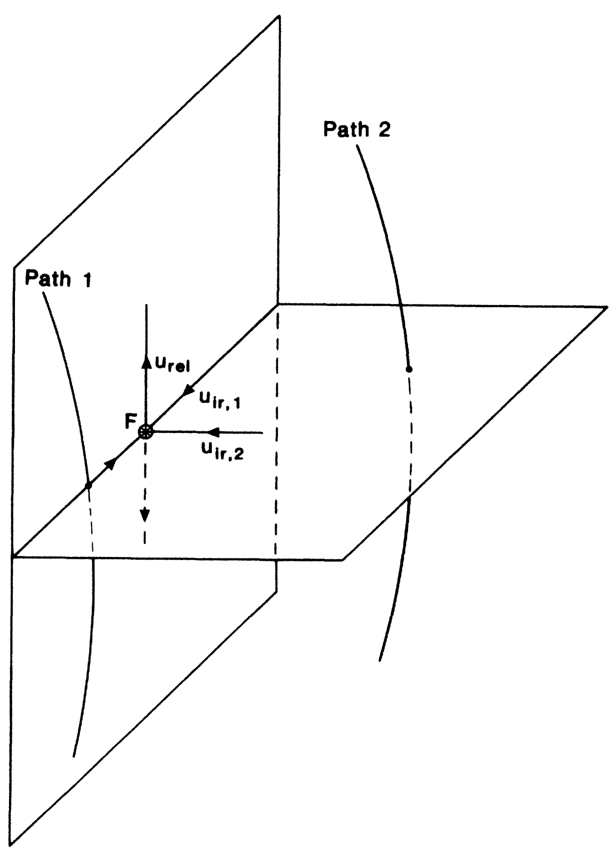

FIG. 1. Phase diagram in the vicinity of the fixed point F, spanned by a relevant (temperature) field, an irrelevant field $u_{ir,1}$ inside the closed conformal block, and an irrelevant field $u_{ir,2}$ outside this block, but still consistent with conformal invariance. Paths 1 and 2 represent models with only conformally invariant interactions, without and with couplings outside the closed conformal block, respectively.

also obey conformal invariance but are outside the closed conformal block, such as the vacancy operator in the Ising case (type 2). In addition one should imagine a fourth direction $u_{ir,3}$ representing nonconformal interactions (type 3). All points in the critical surface spanned by the three types of irrelevant scaling fields belong to the same universality class, i.e., under renormalization each point flows to the fixed point F. Path 1 represents a model, like the nearest-neighbor Ising model, where only corrections to scaling of type 1 are present. Path 2 represents a realization with a microscopic Hamiltonian that obeys conformal invariance, but with contributions from operators outside the closed subalgebra. Finally, realizations that follow the most general type of path (path 3) through the critical surface include nonconformal operators in their Hamiltonian.

Stated this generally, it looks reasonable to expect that models and experimental realizations in general move along paths of type 2 or 3. However, we need convincing explicit examples. All exactly soluble models seem to move along paths of type 1. In this paper we study realizations of the Ising universality class where the vacancy operator must be expected to be present, if it can.

The outline of the paper is as follows. In Sec. II we comment on the finite-size scaling method. In Sec. III we discuss the possible presence of corrections to scaling due to the vacancy operator in a few generalizations of Onsager's model. These are the antiferromagnetic Ising model in a magnetic field (which in the strong-field limit reduces to the hard square model), the Blume-Capel model, and the random cluster formulation of the q-state Potts model around $q=2$. The derivation of the finite-size data for these models, and the search for corrections to scaling due to vacancies, are described in Sec. IV. In Sec. IV A we present the results for the AF Ising model and the hard square problem, and in Sec. IV B the results for the Blume-Capel[16,17] model. In Sec. IV C we show how the vacancy operator comes into play around $q=2$ in the random cluster model. Finally, Sec. V contains our conclusions and comments on other recent work on vacancy corrections to scaling at Ising transitions. Appendix A summarizes a Monte Carlo renormalization analysis of the Blume-Capel model, and Appendix B contains comments on pinninglike phenomena that show up in the behavior of an interface in the case of antiperiodic boundary conditions in the AF Ising model in a field.

II. FINITE SIZE SCALING AND UNIVERSAL AMPLITUDES

It is possible to determine the leading irrelevant exponents accurately from the finite-size scaling behavior of systems with size $n\times\infty$, particularly if the scaling behavior of the leading term is known exactly. For example, the scaling relation for the inverse correlation length associated with the spin-spin correlation function, as a function of a relevant and an irrelevant scaling field,

$$\xi^{-1}(u_{rel},u_{ir},n^{-1})=b^{-1}\xi^{-1}(b^{y_{rel}}u_{rel},b^{y_{ir}}u_{ir},bn^{-1}) , \tag{2.1}$$

implies that at criticality, $u_{\rm rel}=0$, the correlation length scales as a function of the strip width n as

$$\xi^{-1}(0,u_{\rm ir},n^{-1})=n^{-1}(A+B_\xi n^{y_{\rm ir}}+\cdots) \qquad (2.2)$$

This follows by putting $b=n$ in Eq. (2.1) and expanding ξ^{-1} in its second argument. Note that the amplitude B_ξ of the correction-to-scaling term is proportional to the irrelevant scaling field $u_{\rm ir}$. Furthermore, scaling [Eq. (2.1)] implies that the amplitude A of the leading term has the same universal value for all critical points that flow to the fixed point at $u_{\rm rel}=u_{\rm ir}=0$. Moreover, conformal invariance and extended scaling give the exact value of this amplitude, $A=2\pi x_H$ (see, e.g., Nightingale and Blöte,[18] Luck,[19] Derrida and de Seze,[20] and Cardy[4]), where x_H, the critical dimension of the symmetry-breaking field, is equal to $\frac{1}{8}$ for the Ising model.[21] If the universality class is not known in advance, the value of the universal amplitude A may serve as an indicator of the universality class by means of numerical calculations. On the other hand, if the universality class of the transition is not in doubt, it is possible to focus on the finite-size scaling correction to the leading term proportional to A, and determine the leading irrelevant exponent $y_{\rm ir}$ with improved accuracy.

Similarly, we expect the finite-size scaling amplitudes of the surface tension η and the free energy per spin f to be universal:

$$\eta(0,u_{\rm ir},n^{-1})=n^{-1}(2\pi x_H+B_\eta n^{y_{\rm ir}}+\cdots) \qquad (2.3)$$

and

$$f(0,u_{\rm ir},n^{-1})=f_{\rm reg}+n^{-2}(\pi c/6+B_f n^{y_{\rm ir}}+\cdots) \qquad (2.4)$$

(see den Nijs,[22] Blöte *et al.*,[5] and Privman and Fisher[23]). Note that the amplitudes given for the correlation length and surface tension are equal. This is because the inverse correlation length and surface tension are related by means of duality.

In general, it is necessary to specify how the correlation length is determined. Typically the surface tension is given by the difference in free energy between a system with antiperiodic and periodic boundary conditions. The inverse correlation length, on the other hand, is obtained from the ratio of the largest and next largest eigenvalues of the transfer matrix for periodic boundary conditions. The largest eigenvalue is part of the sector of the transfer matrix which is invariant under duality, but the next largest eigenvalue is part of the sector which under duality maps onto the transfer matrix with antiperiodic boundary conditions, and is the largest eigenvalue in this sector. So the surface tension is associated with the order operator O_H, because it is equal to the free energy of an interface between different ordered domains, while the inverse correlation length is associated to the disorder operator. The order and disorder operators have the same critical dimension.[15] However, it is also possible to determine the correlation length associated with a different operator, for instance, by means of the ratio of the two leading eigenvalues of the transfer matrix in the sector which is invariant under duality. In that case the universal amplitude is equal to $2\pi x_T$, i.e., it is associated with the energy operator.

III. MODELS WITH VACANCIES

In order to obtain numerical evidence for the correction-to-scaling exponent $y_{\rm vac}$ in the Ising model, we study several generalizations of the two-dimensional nearest-neighbor Ising model which are likely to contain vacancy excitations. The simplest way to introduce vacancies is to add explicitly an extra spin state $S_i=0$: the spin-1 Ising, or the Blume-Capel model. But vacancies also come into play in the spin-$\frac{1}{2}$ AF Ising model in a magnetic field and in the random-cluster model in the vicinity of the Ising point $q=2$. These three models are briefly introduced, and the role of vacancies in them is discussed in the following three subsections, before we present the numerical results in Sec. IV.

A. The AF Ising model in a field and the hard-square model

We investigate the spin-$\frac{1}{2}$ AF Ising model on the square lattice in the presence of a uniform field h:

$$\mathcal{H}_I=-K\sum_{\langle i,j\rangle}S_iS_j-h\sum_k S_k\ . \qquad (3.1)$$

The phase diagram[24,25] contains an antiferromagnetic critical line, of which only the point at $h=0$ is exactly known. In the limits $h\to\pm\infty$, the critical line is expected to behave like

$$K=-\tfrac{1}{4}|h|+\tfrac{1}{2}\mu_c\ ,$$

where μ is a constant which is not exactly known. It is the critical value of the chemical potential in a hard square model with nearest-neighbor exclusion on the square lattice. Unlike the case exactly solved by Baxter,[26] there are no further interactions between the squares.

The AF Ising model in a magnetic field is applicable to a simple lattice-gas–model description for adsorbed monolayers with two competing commensurate ground states, such as the $c(2\times2)$ ground state of xenon on copper (see Jaubert *et al.*[27] and Schick[28] for a review). The lattice represents the adsorption sites of the substrate. The spin states $S_i=-1$ $(+1)$ represent occupied (empty) sites, and the magnetic field is linearly related to the chemical potential. The two competing ground states of the lattice gas are represented by the AF Ising ground states $(+-)$ and $(-+)$. For $h>0$ vacancy excitations, holes of empty space appear in the ordered phase. In the presence of ferromagnetic next-nearest-neighbor interactions L, these vacancies cause the melting transition to become first order beyond a tricritical point where the density of vacancies becomes too large. In the limit $L\to0$ this tricritical point moves to zero temperature, and at $L=0$ the transition remains critical at all temperatures.[24,25]

Let us summarize three arguments in favor or against completeness of the operator algebra in this model.

(i) The magnetic field controls the density of vacancies, and the enhancement of this topological aspect in the Ising spin configurations should give rise to corrections to scaling. Moreover, the absence of such corrections to scaling in the Onsager solution at zero field might be understood as being caused by the special symmetry at zero field between patches of vacancies $(++)$ and patches of dense areas $(--)$, i.e., spin-up spin-down symmetry.

(ii) Within the wider context of the Potts model, Nienhuis[12] has shown by extended scaling that the leading irrelevant operator associated with these vacancies has a critical dimension $x_{\rm vac}=\frac{10}{3}$ at $q=2$. One can imagine that at $q=2$, i.e., for the case with only two competing ground states, the topology of the vacancies becomes more simple and that, for this reason, the operator with exponent $\frac{10}{3}$ can vanish accidentally. However, the critical exponents at the Ising transition line and at the tricritical point mentioned above are linked to each other analytically within the context of the Potts model and extended scaling. In particular, the crossover operator at the tricritical point in the direction of the critical and first-order lines is the analytical continuation of the vacancy operator at the Ising transitions with exponent $\frac{10}{3}$ that we are looking for. Since the relevant crossover operator $O_{\rm vac}$ is certainly present at the tricritical point, it is hard to imagine how its analytical counterpart at the Ising transition line could remain absent, and not be the operator responsible for moving along the Ising critical line.

(iii) One of the simplest possible pictures that emerges from above arguments is that the fixed point of the Ising critical line is located at zero field and that the crossover operator in the field direction is the vacancy operator we are looking for. It cannot be that simple, however, because in that case the spin-spin correlation function at zero field should include a term with exponent $\frac{10}{3}$. Such a term is absent.[15]

B. The Blume-Capel model

The Blume-Capel model, also known as the Potts lattice gas, is applicable to describe the same monolayer with two degenerate commensurate ground states, by means of spin-1 variables $S_i=1,0,-1$ with ferromagnetic couplings:

$$\mathcal{H}_{\rm BC}=-K\sum_{\langle i,j\rangle} S_iS_j-\Delta\sum_k S_k^2 \ . \tag{3.2}$$

The lattice sites now represent local regions (cells) of the substrate. The states $S=+1,-1$ represent the case that locally the monolayer is in one of the two commensurate ground states, and the vacancy state $S_i=0$ represents the case that locally the substrate is unoccupied.

The fugacity (Δ) controls the amount of vacancy excitations in this model. In analogy with the AF Ising model described in Sec. III A (with a ferromagnetic next-nearest-neighbor interaction included) the phase diagram of Eq. (3.2) includes an Ising critical line and a first-order line separated by a tricritical point, all in the same universality classes as before.[9] We study this model at $\Delta=0$.

For this model the arguments in favor and against completeness are basically the same as for the AF Ising model in a magnetic field, except that argument (iii), which uses perturbation theory around the Onsager solution, does not apply.

C. The random-cluster model

The Ising model is a special case of the q-state Potts model, i.e., $q=2$. The parameter q defines a new direction in which we can search for evidence of the vacancy operator. Thus we check how this operator behaves in the Potts model in the vicinity of $q=2$. We make use of the exact equivalence of the Potts model with the random-cluster model.[29] Starting from the q-state Potts Hamiltonian with only nearest-neighbor interactions,

$$\mathcal{H}_P=-K\sum_{\langle i,j\rangle}\delta_{\sigma_i}\delta_{\sigma_j} \ , \tag{3.3}$$

where σ_i can assume the values $1,2,\ldots,q$, the mapping is achieved by writing the partition function in its high-temperature graphical representation where a factor $\exp(K)-1$ is assigned to each bond in the graph and a factor q to each cluster. The number of Potts spin states q now appears as a parameter in the Boltzmann weight of each graph and can be considered a continuous variable.

The reformulation of the Potts model as the random-cluster model is also the first step in the sequence of mappings used in the extended scaling derivation of the critical exponents of the Potts model (via the six-vertex model to a lattice Coulomb gas). So for arbitrary q we expect that the vacancy operator is present. Also conformal invariance supports the existence of vacancy corrections for $q\neq 2$; only for $q=2$ does the operator algebra close in such a small block that the vacancy operator lies outside. The absence of the vacancy operator in the Onsager solution requires "accidentally" vanishing amplitudes precisely at $q=2$. However, derivatives of finite-size data with respect to q, taken at $q=2$, may be expected to contain vacancy corrections.

IV. NUMERICAL RESULTS

We apply finite-size scaling to several quantities for $n\times\infty$ models described in Sec. III, with cylindrical boundaries. We obtain these quantities by numerical diagonalization of the transfer matrix for $n\leq 16$ in the case of the spin-$\frac{1}{2}$ AF model, and for $n\leq 10$ in the case of the spin-1 and the random-cluster models. The free energy follows from the leading eigenvalue of the transfer matrix, whereas the correlation length is determined by the ratio of the leading and the second eigenvalues. This ratio is negative in the AF models due to the modulation with period 2 of the ground state (it corresponds to the correlation length of the spin-spin correlation function). This technique may now be considered a standard method. Details can be found, e.g., in Refs. 30–33. As the indices of the transfer matrix, we have simply used binary or ternary numbers representing n spins $\frac{1}{2}$ or 1, respectively. The construction of the transfer matrix for the random-cluster model is less trivial because of the presence of nonlocal interactions due to graphs containing arbitrarily long loops. We have made use of an enumeration of "graph connectivities" for the indices of the transfer matrix as constructed in Refs. 33 and 34.

Consider a finite-size quantity $q(n)$ thus obtained numerically for a number of successive system sizes n. The numerical analysis in the following subsections repeatedly involves fitting power-law behavior like

$$q(n)=s+rn^{x}+\cdots .$$

We follow the extrapolation procedure described in Refs. 33 and 35. We require

$$q(m)=s(n,1)+r(n,1)m^{x(n,1)}$$

for three successive values of m, i.e., $m=n$, $m=n+1$, and $m=n+2$; or $m=n$, $m=n+2$, and $m=n+4$ if the finite sizes are restricted to be even. These three-point fits produce a series of estimates $s(n,1)$, $r(n,1)$, and $x(n,1)$ of s, r, and x, respectively. If s is zero, or if $q(n)$ diverges, we can discard the parameter s, so that only two successive values of m are needed instead of three, and the fit reduces to a two-point fit. The second argument ($i=1$) of the fitted parameters $s(n,i)$, $r(n,i)$, and $x(n,i)$ indicates that they are the result of the first step of a procedure that can be iterated; these parameters can again be three-point fitted. For instance, if we want iterated fits $x(n,2)$ of the exponent x, we solve

$$x(m,1)=x(n,2)+t(n,2)m^{u(n,2)}$$

for three successive values of m. These iterated fits are in accordance with the expected[33] power-law convergence of $x(m,1)$.

A. The $S=\frac{1}{2}$ AF Ising model and the $S=1$ Ising model

Since the critical line of the AF Ising model in a field is not exactly known, we have used the scaling relation of the correlation length [Eq. (2.2)] to determine the critical couplings K_c as follows. Finite-size estimates of K_c were obtained for several values of h by solving K from

$$\xi(K,n^{-1})/n=\xi(K,m^{-1})/m \tag{4.1}$$

using data for the correlation lengths associated with the spin-spin correlation function for two consecutive system sizes n and m. For antiferromagnetic models, alternation occurs and only even values of n and m were used. The extrapolation procedure[35] for K_c is described elsewhere. Final estimates of the critical points of the $S=\frac{1}{2}$ models thus obtained are given in Table I. The critical coupling in the hard square limit is in accurate agreement with the series-expansion result of Baxter *et al.*[36]

Analysis of the correlation lengths $\xi(n)$ of strips with finite size n at the critical couplings thus obtained shows that the finite-size amplitudes A defined by Eq. (2.2) for $n\rightarrow\infty$ are accurately equal to the expected universal value[4,18] $\pi/4$. Extrapolated values of A are shown in Table I. These results are in an accurate agreement with Ising universality. Taking universality for granted, we could also estimate K_c by solving K from

TABLE I. Critical couplings K_c of the AF $S=\frac{1}{2}$ Ising model in a field as obtained from the finite-size scaling law of the correlation length, Eq. (4.1). The result for the $S=1$ model is obtained on the basis of Eq. (4.2). Estimated uncertainties in the last decimal places are given between parentheses. The last column gives the extrapolated value of the finite-size amplitude of the correlation length at the values of K_c in the preceding column. These extrapolated amplitudes lie close to the expected value $\pi/4=0.785\,398\ldots$.

Spin	h	K_c	A
$\frac{1}{2}$	0	$-\frac{1}{2}\ln(1+\sqrt{2})$	0.785 40
$\frac{1}{2}$	0.2	−0.444 124(4)	0.785 34
$\frac{1}{2}$	0.5	−0.461 734(4)	0.785 39
$\frac{1}{2}$	1.0	−0.519 652(4)	0.785 42
$\frac{1}{2}$	$\rightarrow\infty$	$-h/4-0.166\,752(3)$	0.785 39
1	0	0.590 473(5)	0.785 40

$$\xi(K,n^{-1})=4n/\pi . \tag{4.2}$$

These estimates are expected to be less vulnerable to numerical inaccuracies. For $S=\frac{1}{2}$, the K_c values from Eq. (4.1) are accurate enough for our purposes, and we did not apply Eq. (4.2).

For the Blume-Capel model, K_c has been determined earlier in Ref. 30 using Eq. (4.1). Again, we reproduce the universal value $\pi/4$ for the universal finite-size amplitude (within a few times 10^{-4}). In this case numerical inaccuracies were noticeable, and Eq. (4.2) yields a significantly more stable result. It is shown in Table I.

Corrections to the leading behavior of ξ^{-1} as given by Eq. (2.2) are generated by irrelevant scaling fields. Consider such fields u_{ir} with exponents y_{ir}. The inverse correlation length depends on u_{ir} as follows:

$$\xi^{-1}(u_{\mathrm{ir}},n^{-1})=\pi/4n+B_{\xi}n^{y_{\mathrm{ir}}-1}+\cdots , \tag{4.3}$$

where we have used $A=\pi/4$. The amplitude B_{ξ} is proportional to u_{ir}. In general, more than one irrelevant scaling field is nonzero, but for large n the correction will be dominated by the least irrelevant scaling field. On the basis of our experiences,[18,22,33] we expect that for finite size 10–16 this asymptotic region will be reached. Therefore we ignore all relevant scaling fields beyond the leading one. The convergence of our numerical results indicates that this is indeed justified.

Two-point fits to ξ^{-1} for the Ising models at the fixed K_c values in Table I yield a clear result: The leading correction is proportional to n^{-3} with an inaccuracy of a few times 10^{-2} in the exponent, corresponding to $y_{\mathrm{ir}}=-2$. This behavior is illustrated in Fig. 2 which shows the quantity

$$Q(n)=n\xi^{-1}(n^{-1})-\frac{\pi}{4}=B_{\xi}n^{y_{\mathrm{ir}}}+\cdots \tag{4.4}$$

versus n on an n^{-2} scale. The linear behavior for large n demonstrates that $y_{\mathrm{ir}}=-2$. It appears that a correction to scaling associated with the expected vacancy exponent $y_{\mathrm{vac}}=-\frac{4}{3}$ is absent.

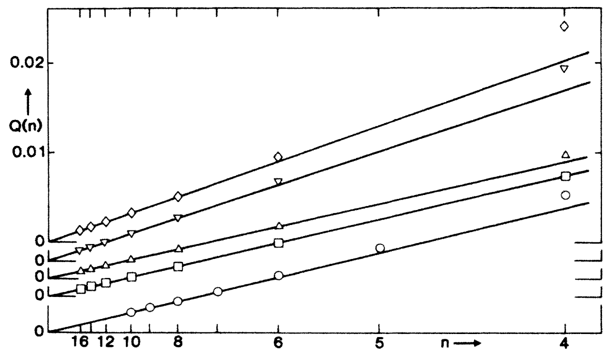

FIG. 2. Corrections $Q(n)$ to the leading finite-size behavior of the inverse correlation length of several Ising models at criticality vs system size n on an n^{-2} scale. Data are shown for the antiferromagnetic Ising model in a magnetic field of strength $h=0.2$ ($\Diamond$), $h=0.5$ (∇), $h=1$ ($\triangle$), and $h=\infty$ ($\square$, the hard square model), and for the Blume-Capel model ($\bigcirc$). These data indicate a correction to scaling exponent $y_{\rm ir}=-2$.

For the free energy per spin $f(u_{\rm ir},n^{-1})$ in the presence of an irrelevant field $u_{\rm ir}$ we expect

$$f(u_{\rm ir},n^{-1})=f_{\rm reg}+\frac{\pi}{12n^2}+B_f n^{y_{\rm ir}-2}+\cdots \tag{4.5}$$

on the basis of Eq. (2.4) and $c=\frac{1}{2}$ for the Ising model. Three-point fits to the quantity $f(n)-\pi/12n^2$ indicate a leading correction term with $y_{\rm ir}=-2$ for all Ising models considered here. Estimates of $y_{\rm ir}$ obtained by means of iterated three-point fits to the free energies of the AF $S=\frac{1}{2}$ models, including the hard square model, are shown in Table II. For the Blume-Capel model, three-point fits show a flat maximum as a function of n (Table III) making iterated fits all but useless for small n. Also in this case $y_{\rm ir}\approx-2$.

We have also obtained some numerical results for the specific heat and the temperature derivative of the correlation length (of spin-spin correlations) by numerical differentiation. Analysis of these quantities also agrees with an irrelevant exponent $y_{\rm ir}=-2$. Besides, the corrections to scaling in the universal amplitude of the surface tension agree with $y_{\rm ir}=-2$ (see Appendix B).

TABLE II. Estimates of the irrelevant exponent $y_{\rm ir}$ of the AF Ising model, obtained from the free energy, for several magnetic field strengths, including $h=\infty$, the hard square model. These estimates are the result of iterated three-point fits to the quantity $f(n)-\pi/12n^2$. Ordinary (not iterated) three-point fits produce a series of estimates which is somewhat longer, but less rapidly convergent (for the largest system sizes these estimates lie between -1.95 and -2.05). An extremum occurs in these estimates for the lower values of h. Missing entries in this table are a consequence of this extremum.

n	$h=0$	$h=0.2$	$h=0.5$	$h=1.0$	$h=\infty$
2	–	–	–	–	−2.18
4	–	–	–	−1.84	−2.01
6	−2.00	−2.00	−2.01	−2.01	−2.01
8	−2.01	−2.01	−2.01	−2.01	−2.00

TABLE III. Estimates of the leading irrelevant exponent $y_{\rm ir}(n,1)$ of the Blume-Capel model as obtained from the free energy by means of three-point fits to the quantity $f(n)-\pi/12n^2$. Due to the presence of an extremum in $y_{\rm ir}(n,1)$ at $n=4$, an iterated fit is meaningful only for $n=6$.

n	$y_{\rm ir}(n,1)$	$y_{\rm ir}(n,2)$
2	−1.43	–
3	−2.10	–
4	−2.32	–
5	−2.30	–
6	−2.26	−1.94
7	−2.16	
8	−2.11	

B. The random-cluster model

The failure of the calculations in the preceding subsection to produce numerical evidence for the vacancy exponent in the Ising model has prompted us to search in a very different direction; namely, to allow q to vary about 2 in the q-state, nearest-neighbor Potts model. Even if amplitudes associated with $y_{\rm vac}$ vanish at $q=2$ (the Ising model), one expects them to show up after a differentiation of the finite-size data with respect to q. Thus we have computed, by means of numerical differentiation along the critical line of the Potts model, the derivatives of the free energies and the correlation lengths of $n\times\infty$ strips of the q-state Potts model at $q=2$. The correlation length calculated here corresponds to the energy-energy correlation function in the Potts model (calculated using the "simple Whitney polynomial" as explained in Ref. 33).

The expansion of the Potts free energy [Eq. (2.4)] in $1/n$ gives

$$f(q,n^{-1})=f_{\rm reg}(q)+\frac{\pi c(q)}{6n^2}+B_1(q)n^{-x_1(q)}+B_2(q)n^{-x_2(q)}+\cdots \,. \tag{4.6}$$

The first[37] and second[5] terms on the right-hand side are exactly known as functions of q. The third term describes a supposed correction with an amplitude that vanishes at $q=2$: $B_1(2)=0$, and an unknown exponent $x_1(q)=2-y_{\rm ir}$. The fourth term is the one found numerically for the Ising model: $x_2(2)=4$.

Thus we have analyzed the quantity

$$\frac{d}{dq}\left[f(q,n^{-1})-\frac{\pi c(q)}{6n^2}\right]_{q=2}$$

by means of three-point fits. We skip the details and only mention the result $x_1(2)\approx+7$.

The absence of an exponent $2-y_{\rm vac}$ in this expansion is, however, not completely unexpected. An earlier analysis[33] of $f(q,n^{-1})$ yielded powers of n close to -2 and -4, and nothing in between, in a range of q values <4.

The situation is different in the case of the correlation length of the Potts model, where nonintegral powers of n do occur[38] for $q \neq 2$. We write the expansion of the inverse correlation length [Eq. (2.2)] as

$$\xi^{-1}(q,n^{-1}) = A(q)/n + a_1(q)n^{y_1(q)-1} + a_2(q)n^{y_2(q)-1} + \cdots . \quad (4.7)$$

The coefficient of the first term on the right-hand side is known from the relation[21] $A(q) = 2\pi x_T(q)$, and the formula due to den Nijs[39,40] for $x_T(q)$. The second term represents a correction due to an irrelevant exponent y_1 and with an amplitude that vanishes at $q = 2$:

$$a_1(2+\epsilon) \sim \epsilon .$$

The third term is the one found in Sec. IV A with an exponent $y_2 = -2$. After bringing the first term to the other side and differentiating with respect to q, we obtain

$$\frac{d}{dq}[n\xi^{-1}(q,n^{-1}) - A(q)]_{q=2} = a_1'(2)n^{y_1(2)} + a_2'(2)n^{-2} + a_2(2)y_2'(2)n^{-2}\ln n + \cdots . \quad (4.8)$$

Primes indicate derivatives to q. One possibility to proceed is to multiply both sides with n^2 and to estimate the exponent $y_1(2)$ in

$$n^2\frac{d}{dq}[n\xi^{-1}(q,n^{-1}) - A(q)]_{q=2} \simeq rn^{2+y_1(2)} + s \quad (4.9)$$

by means of three-point fits. This procedure is expected to work well if $2 + y_1(2)$ is positive and not too small. Table IV shows the results of this procedure. We observe that $y_1 \approx -1.35$, which is close to $-\frac{4}{3}$. Next, we address the question of how the third term in Eq. (4.8) may influence these fits. In the first place we remark that $a_2(2)$ can be obtained numerically from finite-size data for the simple quadratic Ising model: $a_2(2) \approx -5.2$. Unfortunately, we do not know the function $y_2(q)$. It could be independent of q; finite-size data[38] strongly suggest that also at $q = 3$ a contribution is present with $y_2(3) = -2$. But it is likely that the third term in Eq. (4.7) splits up in two terms for $q \neq 2$, one with a constant exponent and the other with an exponent depending on q, causing a logarithmic correction as in Eq. (4.8). In order to investigate the possible effects of such a term, let us for the moment assume that $a_2(2) = -5.2$ and that $y_2(q) = y_T - 3$. This determines the logarithmic term, so that it can be subtracted from both sides of Eq. (4.8). The results for the exponent $y_1(2)$ from subsequent three-point fits is also given in Table IV. The differences with the first column are of the same order as the differences with the expected value $-\frac{4}{3}$. The continuous variation of $y_2(q)$ does not significantly influence the estimate for $y_1(2)$. Another way to obtain the leading irrelevant exponent is by means of iterated two-points fits. The results are also given in Table IV. Again we find $y_1(2) \approx -1.3$. We conclude that $y_1 = y_{\rm vac} = -\frac{4}{3}$ within an accuracy of a few times 10^{-2}.

TABLE IV. The exponent $y_1(2)$ as determined numerically from the finite-size and q dependence of the correlation length of the random-cluster model at $q = 2$. The first column gives the finite-size parameter n, the second gives $y_1(2)$ as estimated by three-point fits (see text). Column three shows the result of the same type of fit after application of a subdominant logarithmic correction. The last column gives the result of iterated two-point fits. These data indicate that corrections to scaling of order ϵ with an irrelevant exponent $y_1(2) \approx -1.3$ arise in the $q = 2+\epsilon$ Potts model. This result agrees well with the predicted value $y_{\rm vac} = -\frac{4}{3}$.

n	3-point	3-point modified	2-point
2	−1.32	−1.40	−1.37
3	−1.37	−1.43	−1.30
4	−1.37	−1.42	−1.29
5	−1.36	−1.41	−1.30
6	−1.36	−1.40	−1.30
7	−1.35	−1.39	−1.30
8	−1.35	−1.39	

V. CONCLUSIONS

In this paper we studied generalizations of the nearest-neighbor Ising model that enhance vacancy excitations. We did not find any evidence for irrelevant operators different than type 1, i.e., those inside the conformal block. At the Ising transitions in the AF Ising model in field, hard square model, and Blume-Capel model the leading irrelevant operator has the critical dimension $x_{\rm ir} = 2 - y_{\rm ir} = 4$. This suggests that also for these generalizations of the nearest-neighbor Ising model the conformal block contains all physically relevant operators.

We found that this does not disagree with extended scaling results, because in the random cluster model the vacancy corrections to scaling are present for continuous q around $q = 2$, with a vanishing amplitude precisely at $q = 2$. It is noteworthy that a very similar accidental vanishing of the amplitude has been found at the self-dual point in the restricted solid-on-solid (RSOS) model.[22] The RSOS model and the body-centered SOS (BCSOS) model both describe surface-roughening transitions. The BCSOS model maps exactly onto the critical line of the Potts model, with q playing the role of temperature in the BCSOS scheme.[39] So $q = 2$ corresponds to a special isolated temperature in the rough phase of the BCSOS model like the self-dual temperature in the RSOS model, where the leading corrections-to-scaling term has zero amplitude.

Also some other recent numerical studies have focused on corrections to scaling in generalized Ising models. Some report evidence for the vacancy exponent $y_{\rm vac} = -\frac{4}{3}$. In particular our results disagree with series results by Adler and Enting[41] for the hard square model. We believe that our method is more accurate, because in the analysis of the series for the magnetization and susceptibility the corrections to scaling only show up as subdominant exponents, while in our approach the leading irrelevant operator determines the dominant finite-size scaling correction to the universal amplitudes (see Sec. II).

Barma and Fisher[42] report evidence for vacancy corrections to scaling from series for slightly different generalizations of the Ising model, i.e., the Klauder and double-Gaussian model. In those models the discrete spin variable is replaced by a continuous variable whose value is controlled by a weight function. It is possible that these generalizations introduce the vacancy operator. However, the authors suggest that their result may mask a logarithmic singularity, while others using somewhat different techniques to analyze the series did not observe the vacancy exponent.[43]

A different possibility to investigate the set of critical exponents is offered by Monte Carlo renormalization. We quote an unpublished study[44] of the $S=1$ Ising model in two dimensions performed recently, using methods developed by Swendsen.[45] The expected exponents y_T and y_H were well reproduced, but unfortunately the leading irrelevant exponents were not well resolved, and no conclusion about the existence of an exponent $y_{\rm ir}=-\frac{4}{3}$ could be drawn. Some further details are given in Appendix A.

Our finite-size scaling results exclude the presence of the vacancy operator in the AF Ising model, hard square model, and Blume-Capel model. The leading irrelevant exponent $y_{\rm ir}=-2$ fits inside the conformal block. This suggests that the operators in this block represent the complete set of operators in these models. It is too early to conclude that corrections to scaling from irrelevant operators of type 2 and 3 (see Introduction) are absent in two-dimensional Ising critical phenomena in general. Actually such a result would be highly surprising. We might have been unfortunate in our selection of generalizations of the nearest-neighbor Ising model. On the other hand, if the paths of type 2 and 3 through the schematic phase diagram of Fig. 1 (see Sec. I) are possible in two-dimensional Ising-like models, how can the models studied here fail to realize them? They explicitly include the topological excitations associated with vacancies.

ACKNOWLEDGMENTS

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APPENDIX A: MONTE CARLO RENORMALIZATION OF THE SPIN-1 ISING MODEL

We summarize the results of an unpublished study by de Bruin, van Leeuwen, and Blöte[44] of the spin-1 Ising model on the square lattice. The additional degree of freedom per spin ($S_i=0$) allows for the introduction of many more interactions under renormalization than for $S=\frac{1}{2}$, i.e., those involving factors S_i^2. It seems reasonable to expect that such an enlargement of the coupling space will introduce additional eigenvalues of the linearized transformation matrix $T_{\alpha,\beta}$. Thus an analysis of the spin-1 model could reveal new irrelevant exponents.

Simulations were performed on lattices up to 64×64; for that size, the simulations had a total length of 350 000 sweeps. Two different block-spin transformations were used: one[46] with a linear scale factor $\sqrt{2}$, and one with a scale factor 2. The analysis, which involved 21 even and 19 odd couplings, reproduced the known magnetic exponent $y_H=\frac{15}{8}$ within a few times 10^{-3}. A second exponent was found to be small and negative, and may be identified with y_H-2. The temperature exponent $y_T=1$ was reproduced with an accuracy of a few times 10^{-2}. In particular the irrelevant thermal exponents were not well determined; these varied considerably with the length of the simulation, with the number of renormalization steps, and with the number of couplings used in the analysis. This inaccuracy is correlated with the occurrence of complex eigenvalues. Probably much longer simulations would be necessary to improve the results. Still, the analyses provided some evidence for an irrelevant thermal exponent close to -1 such as found earlier by Swendsen.[45,47] The calculation with linear scale factor $\sqrt{2}$ provided an indication for another thermal exponent between 0 and -1. Remarkably, no such indications were present in the case that the linear scale factor was 2. No clear information about the values of further irrelevant exponents was obtained. One has to conclude that the accuracy and internal consistency of these Monte Carlo renormalization calculations are such that the question concerning the existence of an exponent $y_{\rm ir}=-\frac{4}{3}$ in the Ising model remains unanswered.

APPENDIX B: PINNING BEHAVIOR IN THE AF ISING MODEL IN A MAGNETIC FIELD

In this Appendix we comment on pinning phenomena of interfaces in the AF Ising model in a magnetic field. Consider a rectangular Ising model with finite size n in the x direction and with size m in the y direction, in the limit $m\to\infty$. The conventional procedure to determine the surface tension in the ferromagnetic case is to compare a ferromagnetic Ising model with periodic (P) boundary conditions, $S(0,y)=S(n,y)$ to a model with antiperiodic (AP) boundary conditions, $S(0,y)=-S(n,y)$, in one direction. AP boundary conditions force an interface into the system, and the free energy of the interface per unit of length is defined as the difference between the free energies of the two systems. AP boundary conditions are obtained from P boundary conditions by reversing the coupling constants $K\to -K$ for all horizontal bonds between spins $S(n,y)$ and $S(1,y)$, i.e., bonds that cross the seam between columns n and 1 where the lattice has been closed to form a cylinder.

It is important to distinguish between the seam and the interface. The interface is the line which intersects the bonds that are actually frustrated. The seam is the line along which the coupling constants have opposite sign in comparison with the bulk. The location of the seam has only a limited physical meaning. In the zero-field Ising model this follows from the invariance of the partition sum under a redefinition of all spins in the strip $n-k<x\leq n$ as $S(x,y)=-S(x,y)$. This transformation moves the seam from $x=k$ to $x=n-k$, but leaves the physics invariant otherwise.

This invariance is lost in the AF Ising model in a magnetic field; the redefinition of the spins changes the direction of the magnetic field for all spins with $x>n-k$. Therefore the determination of the surface tension becomes more complicated. As we will see, in this case both the seam and the interface contribute to the free energy. Moreover, another contribution arises because the interface shows pinning behavior with respect to the seam.

The phase diagram of the model (3.1) is symmetric, and we restrict ourselves to the case $h\geq 0$. Figure 3 shows several zero-temperature configurations for even strip width n both for P and AP boundary conditions. Figure 4 illustrates the different case that n is odd. For odd n and P boundary conditions [Fig. 4(a)] only the interface is present; for odd n and AP boundary conditions [Fig. 4(b)] only the seam is present, while for even n and AP boundary conditions [Fig. 3(b)] both the seam and interface are present. Therefore the free energy of the interface, the free energy of the seam, and the pinning free energy, which measures the attraction between the interface and the seam per unit of length, are given as

$$f_{\mathrm{int}}(n)=\lim_{m\to\infty}[F_{\mathrm{P,odd}}(n,m)-F_{\mathrm{P,even}}(n,m)]/m$$

$$f_{\mathrm{seam}}(n)=\lim_{m\to\infty}[F_{\mathrm{AP,odd}}(n,m)-F_{\mathrm{P,even}}(n,m)]/m$$

$$f_{\mathrm{pin}}(n)=\lim_{m\to\infty}[F_{\mathrm{AP,even}}(n,m)+F_{\mathrm{P,even}}(n,m)-F_{\mathrm{P,odd}}(n,m)-F_{\mathrm{AP,odd}}(n,m)]/m\ ,$$

where the quantities $F_{*,\mathrm{even}}$ and $F_{*,\mathrm{odd}}$ ($*=$AP or P), which are, strictly speaking, defined only for even and odd values of n, respectively, are obtained by interpolation where necessary.

The zero-temperature configurations in Figs. 3 and 4 demonstrate that at very low temperatures and small magnetic field the interface does not interact strongly with the seam; compare the energies of Figs. 3(b1), 4(a1), and 4(b1). However, for sufficiently strong magnetic fields (including the hard square model) the interface prefers to coincide with the seam [see Fig. 3(b4)]. Thus, the interface changes of character near the line $h/K=-2$.

At small h, compare Fig. 3(a1) with 4(b1), the seam does not cost energy at zero temperature; there are no frustrated bonds and the magnetization in the columns adjacent to the seam is equal to that in the bulk. However, a thermal excitation that flips two nearest-neighbor spins is easier at the seam than in the bulk [see the spin

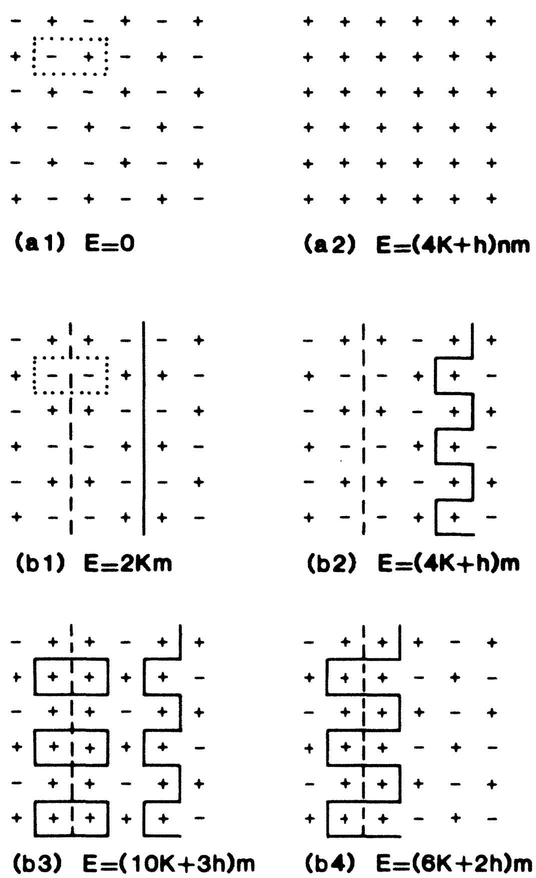

FIG. 3. Low-temperature spin configurations of the antiferromagnetic Ising model in a magnetic field for (a) periodic and (b) antiperiodic boundary conditions, for a strip of even width n (horizontal) and length m. The factor $-1/kT$ has been absorbed in the energies E. Therefore, the ground state has the highest value of E. All energies are given relative to the antiferromagnetic ground state (a1). The dashed line represents the seam and the solid line the interface between the two AF ground states. For $h>-2K$ the interface is attracted by the seam; see (b1), (b2), and (b4).

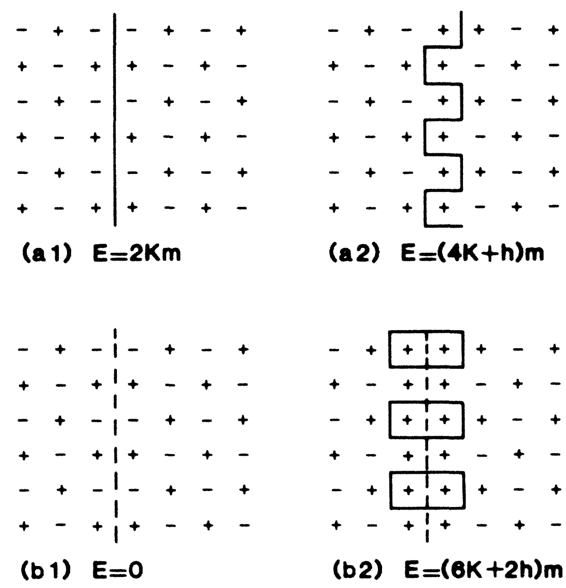

FIG. 4. Zero-temperature spin configurations as in Fig. 4, but now for odd strip widths n. Now only an interface (solid line) is present for P boundary conditions, and only a seam (dashed line) for AP boundary conditions.

pairs surrounded by dotted lines in Fig. 3(a1) and 3(b1)]. So the seam starts to gain free energy at nonzero temperatures. The seam plays a role similar as a line defect in the zero-field Ising model. The magnitude of the line defect increases with h as a consequence of the field dependence of the aforementioned interaction between the seam and the interface. The system with a seam can be compared to a zero-field Ising model with a line defect that consists of a column of horizontal bonds with a reduced strength. Obviously such a line defect would also attract an interface. Investigations of line defects in the Ising model[48,49,35] have shown that the defect operator is marginal; nonuniversal behavior occurs as a function of the magnitude of the defect. So the free energy of the seam is likely to include an independent defect exponent $y_{\rm def}$. Therefore we expect the following scaling behavior for $f_{\rm int}$ and $f_{\rm seam}$ at criticality:

$$f_{\rm int}(n)=n^{-1}(A_i+B_i n^{y_{\rm ir}}+\cdots),$$

$$f_{\rm seam}(n)=f_{\rm seam}(\infty)+B_s n^{y_{\rm ir}-1}+B_d n^{y_{\rm def}-1}+\cdots$$

with universal amplitude $A_i=2\pi x_H$ (see Sec. II).

We have determined the finite-size scaling behavior of these quantities in several points on the critical line. The even free energies for odd n are defined as

$$\frac{1}{m}F_{*,\rm even}(n,m)=\frac{1}{2m}[F_{*,\rm even}(n-1,m)+F_{*,\rm even}(n+1,m)]-\frac{\pi}{12n^3}.$$

The last term neutralizes the leading-order effect due to the averaging of the nonlinear function $\pi/12n$: the universal finite-size contribution to the free energy. This should work well for $F_{\rm P,even}$ where contributions due to an interface or a seam are absent.

Finite-size analysis of the interface free energy[38] confirms that $f_{\rm int}\simeq A_i/n$ with $A_i=-\pi/4$ within a few times 10^{-5}. We obtained two-point fits for

$$nf_{\rm int}(n)+\pi/4\simeq B_i n^{y_{\rm ir}}.$$

TABLE V. Estimates of the exponent $y_{\rm ir}$ for the surface tension in the AF Ising model in a magnetic field, according to $nf_{\rm int}(n)=\pi/4+a_i n^{y_{\rm ir}}$. The finite-size data for the interface energy were obtained from the free-energy differences between systems with odd and with even finite size as explained in the text. These data confirm that $y_{\rm ir}=-2$ in the Ising model.

n	$h=0$	$h=0.2$	$h=0.5$	$h=1.0$	$h=\infty$
3	-2.48	-2.45	-2.51	-2.61	-1.33
5	-2.74	-2.50	-2.45	-2.44	-1.77
7	-2.25	-2.24	-2.24	-2.24	-1.86
9	-2.14	-2.13	-2.14	-2.16	-1.89
11	-2.09	-2.07	-2.09	-2.12	-1.92
13	-2.07	-2.03	-2.06	-2.11	-1.93

Estimates of $y_{\rm ir}$ are given in Table V. Although some numerical inaccuracy is apparent, probably due to the finite accuracy of our K_c estimates, the data clearly indicate that $y_{\rm ir}\approx-2$ along the entire critical line, in agreement with the results in Sec. IV A.

Next, we have applied three-point fits to $f_{\rm seam}(n)$. The constant $f_{\rm seam}(\infty)$ was clearly resolved. Numerical values are shown in Table VI. We see that $f_{\rm seam}(\infty)$ is positive; it represents indeed a gain in free energy. Its value is approximately proportional to h^2. The finite-size dependence of $f_{\rm seam}(n)$ is rather small and not monotonic; no accurate value of the correction-to-scaling exponent was produced. This may have to do with the marginal operator in Ising models with a line defect.[48,49,35]

Finally we studied the pinning behavior along the critical line. One might expect to find along the critical line a point W (Fig. 5) at some field h_W such that for $0\le h\le h_W$ the interface is free from the seam until criticality and for $h>h_W$ remains bound to the seam until criticality. There exists a familiar argument by Cahn[50] which applies to wetting phenomena and implies that the critical fluctuations always cause the interface to unbind from a wall-type attractor before the critical line is reached, i.e., that point W in Fig. 5 would be located at

TABLE VI. Estimates $y_{\rm pin}(n,k)$ of the exponent $y_{\rm pin}$ in the AF Ising model in a magnetic field as determined from the finite-size dependence of the pinning free energy, for $k=1$ (two-point fits) and for $k=2$ (iterated fits). Only for $h\ge0.5$ do we observe signs of convergence; these results suggest $y_{\rm pin}=0$. The lowest row gives the energy of the seam per unit of length. Estimated uncertainties in the last decimal place are given between parentheses. The bottom line contains the extrapolated values of $f_{\rm seam}$ at these values of h.

n	k	$h=0$	$h=0.2$	$h=0.5$	$h=1.0$
5	1	-2.033	-3.79	–	0.90
7	1	-2.017	-4.09	1.49	0.42
9	1	-2.011	-12.09	0.76	0.27
11	1	-2.007	–	0.49	0.19
13	1	-2.005	3.95	0.35	0.15
5	2	-2.001	–	–	0.12
7	2	-2.000	–	0.21	0.06
9	2	-2.000	–	0.10	0.04
$f_{\rm seam}(\infty)$		$<10^{-7}$	0.002 025(5)	0.012 80(2)	0.053 28(2)

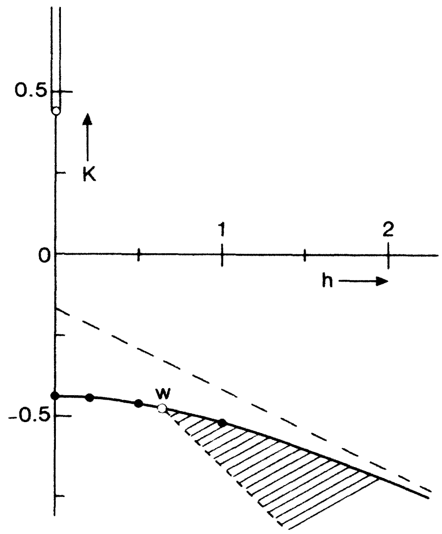

FIG. 5. Phase diagram of the simple quadratic Ising model with nearest-neighbor coupling K in a magnetic field h. Only the right-hand side of the diagram is shown; it is symmetric with respect to change of sign of h. Finite-size calculations are performed in several points (solid circles) on the antiferromagnetic critical line, including the point at $h=\infty$ indicated by the asymptote (dashed line) of the critical curve. The open circle shows the possible location of the point W (see text). At least for sufficiently large h, the interface is pinned to the seam (shaded area).

$h \rightarrow \infty$. However, in our case the seam represents a different type of attractor, with respect to which the interface can fluctuate on both sides. One expects that such an interface remains pinned until criticality as long as the effective interaction between the seam and the interface is attractive (see, e.g., van Leeuwen and Hilhorst[51]). This is obviously the case for $h/K < -2$, at least at low temperatures. So the remaining question is whether entropy leads to an effective attraction or repulsion between the interface and the seam, in particular for $h/K > -2$.

In the hard square limit the interface is always pinned. The spins in the columns adjacent to the seam freeze into the $S=+1$ state; the AP boundary condition acts as an open boundary condition with frozen boundary spins. Moreover, Figs. 3(b4) and 4(b2) look almost the same. The only difference is that the further neighbor spins $S=-1$ across the seam are opposite to each other in the presence of the interface, Fig. 4(b2), but shifted in Fig. 3(b4). The important point is that the interface does not contribute to the energy as long as it remains merged with the seam. The free energy of the seam in Fig. 4(b2) and of the seam plus interface in Fig. 3(b4) are equal, because the only fluctuations which contribute to the difference are those where the spins at the seam fluctuate into the $S=-1$ state; these fluctuations are frozen out in the hard-square limit. So the interface remains pinned to the seam until criticality; Cahn's argument does not apply. Moreover, $f_{\text{pin}}(n)=-f_{\text{int}}(n)\rightarrow 0$ at the critical point.

The finite-size scaling behavior of f_{pin} can, in principle, resolve the location of W. We consider three different cases in the ordered phase of a system with AP boundaries:

(a) $f_{\text{pin}}=0$ in the region where the interface is unbound.

(b) For n even, pinning occurs when the seam and the interface form a bound state with free energy $f_{\text{bound}} > f_{\text{seam}} + f_{\text{int}}$; the pinning free energy $f_{\text{pin}} = f_{\text{bound}} - f_{\text{seam}} - f_{\text{int}}$ is positive. Furthermore, we restrict the case (b) by the additional condition $f_{\text{bound}} < f_{\text{seam}} - f_{\text{int}}$. If this condition is violated, states with a seam but without an interface [see Figs. 4(b)] become unstable as explained under (c).

(c) When pinning is so strong that the condition $f_{\text{bound}} < f_{\text{seam}} - f_{\text{int}}$ is no longer satisfied, two interfaces will spontaneously be created in systems with odd n and AP boundary conditions [see Figs. 4(b)]. One of these forms a bound state with the seam. Adhering to the definition of f_{seam} given earlier, $f_{\text{bound}} = f_{\text{seam}} - f_{\text{int}}$, so that $f_{\text{pin}} = -2f_{\text{int}}$.

Moving now to the critical line, we can consider the following finite-size scaling form for $f_{\text{pin}}(n)$:

$$f_{\text{pin}}(n) = f_{\text{pin}}(\infty) + B_p n^{y_{\text{pin}}-1} .$$

In the unbound case, corresponding to (a), $f_{\text{pin}}(n)$ must scale to zero faster than f_{int}, i.e., $f_{\text{pin}}(\infty)=0$ and $y_{\text{pin}}<0$. Along a bound section of the critical line corresponding to case (b), $f_{\text{pin}}(\infty)=f_{\text{bound}}-f_{\text{seam}}$. However, since $-f_{\text{int}} \geq f_{\text{bound}} - f_{\text{seam}} > f_{\text{int}}$ and $f_{\text{int}} \approx 2\pi x_H/n \rightarrow 0$, this case can only appear if $f_{\text{bound}} - f_{\text{seam}} \rightarrow 0$ at criticality at a rate faster or equal than f_{int}. So $f_{\text{pin}}(\infty)=0$, $y_{\text{pin}}=0$, and $B_p>0$. Moreover, if $f_{\text{bound}}-f_{\text{seam}}$ scales faster to zero than n^{-1}, the leading power law only reflects the scaling behavior of f_{int}, i.e., $B_p = 2\pi x_H$. Finally, in the pinned case corresponding to (c), where $f_{\text{pin}} = -2f_{\text{int}}$, we have $f_{\text{pin}}(\infty)=0$, $y_{\text{pin}}(\infty)=0$, and $B_p = 4\pi x_H$. Thus in all cases $f_{\text{pin}}(\infty)=0$. The difference between the free and pinned portions of the critical line is signaled by the value of the critical exponent y_{pin}. Notice that the hard square limit, discussed earlier, corresponds to case (b). Our present numerical data do not converge sufficiently well to draw a definite conclusion about the location of W. For $h>0.5$ (see Table VI) the convergence is consistent with $y_{\text{pin}}=0$, suggesting a location of W at $0 \leq h < 0.5$.

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